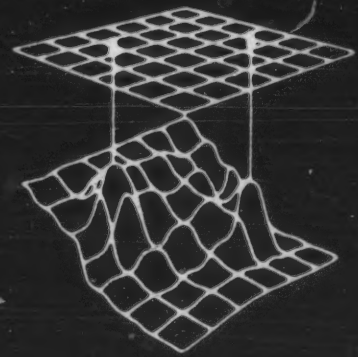




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**Development of
Techniques for Fast Field-Scale
Simulation of Gas-Injection Processes**

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PREFACE

This report describes the research results in the project entitled "Development of Techniques for Fast Field-Scale Simulation of Gas Injection Processes," during the period April 1, 1990 to March 31, 1991 as part of the CANMET Energy Conversion Cost-Shared Program 1990/1991.

EXECUTIVE SUMMARY

This report describes techniques for speeding up compositional simulation such that it can be used routinely in large field-scale simulation. The techniques investigated in this report consist of:

1. The reduction of the number of components required to represent the hydrocarbon system.
2. The development of K-value correlations consistent with the equation of state.
3. The investigation of a general flash calculation algorithm that would allow rapid detection of single-phase mixtures.
4. The proper selection of timestep size that would optimize the number of implicit gridblocks and consequently the run-time.

It was found that the reduction of components has the largest impact on run time. The K-value correlations are useful for systems with a large number of components (ten or more). The general flash calculation performs competitively against the current flash calculations with stability tests, and allows a much simpler code. The optimal timestep selection based on stability criteria yields only marginal improvements over current compositional techniques. In the process of investigating the general flash calculation algorithms, a flash calculation procedure for systems with any number of phases was also developed.

SOMMAIRE EXÉCUTIF

Ce rapport décrit des techniques pour accélérer la simulation compositionnelle tel que celle-ci peut être utilisée fréquemment dans les grandes simulations des gisements d'hydrocarbures. Les techniques examinées dans ce rapport sont:

1. La réduction du nombre de composants requis pour représenter le système d'hydrocarbures.
2. Le développement des corrélations pour les constantes d'équilibre qui sont compatibles avec l'équation d'état.
3. L'investigation d'un algorithme pour le calcul d'équilibre général qui permet une détection rapide des mélanges monophasiques.
4. La sélection adéquate des pas de temps dans la simulation qui optimise le nombre de mailles implicites et conséquemment le temps d'exécution.

On a trouvé que la réduction du nombre de composants a le plus grand effet sur le temps d'exécution. Les corrélations des constantes d'équilibre sont utiles pour les systèmes renfermant un grand nombre de composants (dix ou plus). Le calcul d'équilibre général est compétitif avec le calcul d'équilibre courant qui utilise le test de stabilité, et a un code plus simple que ce dernier. La sélection optimale des pas de temps basée sur les critères de stabilité donne seulement des améliorations marginales sur les techniques compositionnelles courantes. En développant le calcul général d'équilibre, on a découvert une procédure pour le calcul d'équilibre des systèmes multiphasiques avec un nombre quelconque de phases.

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1. INTRODUCTION

Compositional simulators which utilize an equation of state are state-of-the-art tools for predicting processes where the hydrocarbon phase behavior is complex. Examples of problems requiring compositional simulators are: (1) primary production or cycling of gas condensate reservoirs, and (2) enhanced oil recovery by injection of enriched gas or CO₂.

Although compositional simulators provide a comprehensive predictive technique for gas-injection processes, they have not been widely used in large field-scale simulation involving thousands of gridblocks because of the substantial computational time involved. This is caused by: (1) the large number of components required to model the hydrocarbon system (often more than ten), (2) the complexity of flash calculations with the equation of state, (3) the timesteps used during a simulation that may require unnecessarily large numbers of implicit gridblocks and Newtonian iterations.

In this project it is proposed to investigate and develop techniques that address the above issues. This involves:

- (1) The investigation and development of techniques to minimize the number of components required to model the hydrocarbon system (Tasks 1 and 2 of the work statement).
- (2) The investigation and development of K-value correlations that are consistent with the equation of state (Task 3).
- (3) The investigation of techniques for a rapid detection of single-phase regions without invoking stability-test calculations (Task 4).
- (4) The investigation of techniques for optimizing timestep sizes during a simulation (Task 5).

2. OPTIMAL REPRESENTATION OF HEAVY FRACTIONS IN THE SIMULATION OF MULTIPLE-CONTACT PROCESSES

2.1 Introduction

Rich-gas and CO₂ injection are important enhanced-oil-recovery processes, where multiple contacts between the injected gas and the reservoir oil result in efficient displacement of oil. The traditional interpretation of the mechanisms occurring in rich-gas drive corresponds to a condensing process where the intermediate components condense from the injection gas and enrich the reservoir oil towards the point of miscibility (Stalkup, 1984). However, recent studies indicate that the mechanisms in most rich-gas drives correspond to a combined condensing/vaporizing phenomena or a liquid-extraction phenomena (Zick, 1986; Mansoori and Gupta, 1988; Novosad and Costain, 1988, 1989). Thus, the phenomena which occur in rich-gas drives are in many ways similar to those in CO₂ processes (Novosad and Costain, 1989).

The above phenomena are usually modelled with a cubic equation of state (EOS). With this approach, the number of components representing the hydrocarbon system has a large impact on accuracy and computational cost. The computational costs are an overriding factor if EOS calculations are used in a compositional simulator to predict reservoir performance. Thus, it is essential to reduce the number of components in field-scale simulation, while still preserving the accuracy of the phase behavior predictions.

The most important factor in reducing the number of components is the representation of the heavy fraction (e.g. C₆₊) of the reservoir fluid. A number of methods have been proposed to split the heavy fraction into several pseudocomponents and to characterize these pseudocomponents. This characterization involves the estimation of component critical properties and acentric factors. Some of these techniques are described in Whitson (1983), Pedersen et al (1984), Li et al (1985), Coats and Smart (1986), Wu and Batycky (1988), and Newley and Merrill (1989). These techniques usually require a sizeable number of pseudocomponents to represent the heavy fraction (four or more) in order to obtain accurate predictions of the phase behavior of multiple-contact processes. Although there were reports of some success of using one or two pseudocomponent for the heavy fraction (Coats and Smart, 1986; Wu and Batycky, 1988), a close examination of these papers reveals that the processes that were modelled were mainly constant-composition and constant-volume expansion of reservoir oils and gas condensates (Coats and Smart, 1986) and condensing-gas processes (Wu and Batycky, 1988). The modelling of condensing/vaporizing phenomena or liquid-extraction phenomena reported in the literature (Zick, 1986; Stalkup, 1987; Mansoori and Gupta, 1988; Novosad and Costain, 1988, 1989; Newley and Merrill, 1989) required four or more pseudocomponents to represent the heavy fraction.

This section presents a novel technique for representing the heavy fraction of reservoir fluids that allows the modelling of multiple-contact processes (including condensing/vaporizing processes) with one or two components. Before elaborating on the technique, it is useful to describe briefly the mechanisms which occur in multiple-contact processes.

2.2 Multiple-Contact Process Mechanisms

The combined condensing/vaporizing mechanism for oil recovery in rich-gas injection was first proposed by Zick (1986). He showed that in this process there is a region where light intermediates (C₂ to C₅) from the solvent condense into the oil and there is also a region where heavy components (C₆₊) are vaporized into the gas phase. The representation of this process on a

pseudoternary diagram shows an hourglass-shaped two-phase region as depicted in Figure 2.1a. There is a transition between the vaporizing and condensing regions where the oil and gas properties converge, giving rise to low interfacial tensions (IFT). The lowest IFT corresponds to the minimum tie-line length (Mansoori and Gupta, 1988). High displacement efficiency can be obtained in this region without miscibility. This explains the high recovery obtained in many rich-gas processes without the attainment of true miscibility. These high recoveries cannot be explained by the traditional condensing gas-drive concept. As pressure increases, the two-phase envelope shows much more of a constriction (Figure 2.1b) indicating a further reduction of IFT. As pressure further increases, this low IFT region can pinch out yielding two separate two-phase regions. However, in the multiple-contact process between the rich gas and the reservoir oil only one two-phase region is meaningful as depicted in Figure 2.1c. This then can give rise to miscibility between the reservoir oil and injection gas through a vaporization or liquid-extraction process. This latter mechanism was highlighted by Novosad and Costain (1988, 1989).

For CO₂ processes, the mechanisms are similar. Larsen et al (1989) reported ternary diagrams for CO₂/C₁/C₁₆ mixtures, which are analogous to the ternary diagrams in Figure 2.1 except that CO₂ replaces the intermediate components in the upper apex of the diagrams. These mixtures are representative of fluid systems encountered in CO₂ floods. Some minor differences in the diagrams can be observed. At low pressures, the two-phase region forms a band stretching across the ternary diagram. As the pressure increases, a constriction in the phase envelope occurs as in the rich-gas process (Figure 2.1b). If the reservoir temperature is close to the critical temperature (T_c) of CO₂ (31°C or 88°F), a three-phase liquid/liquid/vapor system may form in the constricted region. In this region, the extraction (liquid-extraction process) of heavy components by the CO₂-rich phase is efficient giving rise to low IFT. As the pressure further increases, the phase envelope becomes similar to Figure 2.1c. If the reservoir temperature is much higher than the critical temperature of CO₂, the second liquid phase may not appear and the extraction process is more appropriately called a vaporization process.

The pressure-composition diagram of a reservoir oil/injection gas system is a valuable tool to help identify the process mechanisms. For a condensing/vaporizing process, the pressure-composition diagram has a critical point to the left of the maximum pressure (cricondenbar) as shown in Curve 1 of Figure 2.2. This curve usually applies to rich-gas injection. Curve 2 in Figure 2.2 represents the pressure-composition diagram of a typical reservoir oil/injection gas system corresponding to a vaporizing (or liquid-extraction) process. This curve is typical of reservoir oil/CO₂ mixtures.

2.3 Pseudocomponent Representation of Heavy Fraction

The sizeable number of components used to represent the heavy fraction reported in the literature is probably due to the complex mechanisms associated with the condensing/vaporizing process. Zick (1986), Mansoori and Gupta (1988) and Novosad and Costain (1989) reported that the use of one pseudocomponent is normally sufficient to model the traditional condensing phenomena.

A technique is proposed here that allows the representation of the heavy fraction by very few pseudocomponents (one or two). The highlights of the technique proposed in this paper are:

- a) the T_c of the pseudocomponent representing the heaviest pseudocomponent is allowed to vary with composition. It is anticipated that allowing the T_c of the heaviest pseudocomponent to vary would adjust the K-values of the few-component system to reproduce the phase behavior exhibited by the many-component system.

- b) the pseudocomponents were characterized such that they yield a critical point on the pressure-composition diagram (if it exists) similar to the one predicted by the many-component system. This is crucial for the system to exhibit a condensing/vaporizing phenomenon as opposed to the traditional condensing phenomenon.

2.4 Approach

Two examples, one of a CO_2 vaporizing process and the other of a rich-gas condensing/vaporizing process are used to demonstrate the technique. These processes correspond to systems with pressure-composition diagrams illustrated in Figure 2.2. All calculations were performed with the Peng-Robinson (1976) EOS.

Initially, a detailed description of a typical reservoir oil was obtained from published data. The oil was split into 14 components including 5 pseudocomponents for the heavy fraction. This representation will be referred to as the many-component representation. These component properties (critical pressure p_c , critical temperature T_c , interaction coefficients) were adjusted to match experimental data which may include saturation pressures, constant composition expansion data, and multiple contact data. The regression procedure of Agarwal et al (1990) was used in the data matching.

After this matching of the experimental data, the saturation pressures of mixtures consisting of various proportions of reservoir oil and injection gas (static mixtures of 0 mole % to 90 mole % injection gas) were calculated to generate the pressure-composition diagram for the many-component system. Multiple-contact calculations were also performed at a pressure representative of the flooding pressure.

The many-component system was then reduced to a system with fewer components. Regression was performed by varying the T_c of the heaviest pseudocomponent to match the saturation pressures and the multiple-contact results (phase splits and K-values) obtained with many components. A key component was defined (e.g. CO_2 in CO_2 floods and C_3 or $\text{C}_2\text{-C}_3$ in rich-gas flooding), and regression was performed separately for each key-component composition. This yields the desired variation of T_c of the heaviest pseudocomponent with respect to the mole fraction of the key component. In the regression, more emphasis is given to the matching of the multiple-contact results than the saturation pressures, especially at very high concentrations of injection gas since this region was found to be unimportant in the displacement process. If satisfactory matches of the multiple-contact phase behavior or the pressure-composition diagram could not be obtained, the number of pseudocomponents used to represent the heavy fractions was increased and the regression procedure was repeated.

Finally, multiple-contact calculations were performed with the few-component system. The results were plotted on pseudoternary diagrams and compared with the many-component predictions. Multiple-contact calculations were also performed at a pressure different from the multiple-contact pressure where the regression was performed in order to check the validity of the technique when the pressure changes. In addition to multiple contact calculations, slim tube simulations were also performed to compare recovery obtained with the many- and few-component systems.

2.5 CO₂ Vaporizing Process

Sigmund et al (1979) reported phase-behavior data for a CO₂/reservoir oil system. The compositions and saturation pressures of the recombined reservoir fluid and four mixtures of the reservoir fluid with CO₂ are shown in Table 2.1. A 14-component system was used to represent the oil with 5 components for the C₆₊ fraction (Table 2.2). The bubble-point pressures calculated with 14 components are reported in Figure 2.3 showing good agreement with the experimental data. Note that the 14-component system was able to model the very steep rise in saturation pressure above 60 mole % CO₂ and was able to predict the saturation pressure at 78% accurately. In order to achieve this match at the 78 mole % CO₂, the saturation pressures at lower concentrations of CO₂ were not as accurate. This pressure-composition diagram indicates a vaporizing process. Multiple-contact calculations were then performed with 14 components at 15 000 kPa [2176 psia]. The corresponding pseudoternary diagram is shown in Figure 2.6.

The 14-component system was reduced to a 4-component system, which is also shown in Table 2.2. Note that the C₆₊ fraction is represented by only one pseudocomponent. In order to match the 14-component saturation pressures and multiple-contact results, the T_c of the C₆₊ pseudocomponent is allowed to vary with the global composition of CO₂ as discussed previously. Regression yielded a curve of T_c of C₆₊ versus CO₂ composition as illustrated in Figure 2.4. This curve was obtained by regression using the multiple-contact phase splits and K-values as well as the static mixture saturation pressures. This gave an excellent match of the multiple contact phase compositions and a good match of static mixture saturation pressure. For global CO₂ concentrations of 50 mole % or less the critical temperature of the C₆₊ fraction for the four component system decreased roughly linearly with CO₂ mole %. Above 50% CO₂ the critical temperature was constant. A comparison of the calculated saturation pressures for the 14- and 4-component systems is shown on Figure 2.3. Good agreements between the two systems were obtained for CO₂ concentrations less than 60 mole %. Some discrepancies occur for higher concentrations of CO₂. For these high CO₂ concentrations, the saturation pressure curve is very steep and an exact match would require changing substantially the critical temperature of the C₆₊. As mentioned earlier, more emphasis was given to the matching the composition of the multiple-contact equilibrium phases. Furthermore, the region of high concentration of injection gas is not important in the prediction of the multiple-contact recovery. An excellent match of the C₆₊ composition for the oil phase along the saturation curve with 14 and 4 components was also obtained as depicted in Figure 2.5.

Several other CO₂-oil systems with similar pressure-composition diagrams to the Sigmund et al. (1979) system were also studied, and very similar results were obtained. One pseudocomponent for the heavy hydrocarbon fractions was found to be sufficient for all cases, and a total of four to five pseudocomponents was adequate for the whole mixture. The trend of the critical temperature of the heavy fraction versus CO₂ concentration was also similar, decreasing linearly with CO₂ concentration at low and intermediate concentrations and remaining constant at higher concentrations of CO₂.

Multiple-contact calculations were performed at 15 000 kPa [2176 psia] and 19 000 kPa [2756 psia] with both the 14-component and 4-component system. Figures 2.6 and 2.7 show the corresponding pseudoternary diagrams. An excellent match between the two systems was obtained. Although the C₆₊ T_c's were obtained from multiple-contact results at 15 000 kPa [2176 psia], the excellent agreement at 19 000 kPa [2756 psia] indicates that this technique is also valid as pressure changes, which is a very important consideration for the practical application of the technique.

2.6 Rich-Gas Condensing/Vaporizing Process

Calculations were performed with the reservoir oil of Sigmund et al (1979) described above and a rich gas with the following composition: 30 mole % C_1 , 40 mole % C_2 and 30 mole % C_3 . The oil/rich-gas system was initially modelled with 14 components shown in Table 2.2. The pressure-composition diagram for this system is shown in Figure 2.8. The critical point is to the left of the cricondenbar, which indicates a condensing/vaporizing process. The 14-component system was reduced to a 6-component system also reported in Table 2.2. For rich gas/reservoir oil systems more components are usually required because the methane (C_1) must be kept as a separate component and the C_{2+} in the solvent must be added as another component. In addition, for a condensing/vaporizing mechanism, two pseudocomponents may be required to model the vaporization of the heavy fraction accurately. For this example, two C_{6+} pseudocomponents were indeed needed. A preliminary attempt to use only one pseudocomponent for C_{6+} was not successful because it failed to give a critical point on the pressure-composition diagram for any value of T_c of the C_{6+} (only a bubble-point curve was predicted, no dew-point curve was predicted). The predictions with one C_{6+} pseudocomponent always gave a closed pseudoternary diagram indicating a condensing process as noted by Zick (1986). Although two pseudocomponents were used for C_{6+} , only the T_c of C_{13+} was allowed to vary with composition. Regression using the pressure-composition diagram and multiple-contact results at 15 000 kPa [2176 psia] yielded the C_{13+} T_c 's shown in Figure 2.9. The trend is very similar to the previous case (Figure 2.4) with the critical temperature initially decreasing almost linearly with global solvent composition and then becoming constant at higher concentrations of solvent. Figure 2.8 shows the calculated pressure-composition diagram for the 14-component and 6-component systems. Very good agreement between the two systems was obtained. Note that the 6-component system gave a critical point on the pressure-composition diagram very close to that of the 14-component system. Figure 2.10 shows the excellent match between the two systems of the C_{13+} concentration in the oil phase on the saturation curve.

Figures 2.11 and 2.12 show the results from multiple-contact calculations at 15 000 kPa [2176 psia] and 19 000 kPa [2756 psia]. These diagrams are typical of the condensing/vaporizing phenomena illustrated in Figure 2.1a and 2.1b. Almost identical results were obtained for the 14-component and the 6-component system. For illustrative purposes, the multiple-contact results obtained with one pseudocomponent for C_{6+} (6 pseudocomponents for the whole mixture) is shown in Figure 2.13. The results show a closed two-phase region, indicating a conventional multiple-contact miscible condensing gas drive process. This is quite different from the hourglass-shaped two-phase region in Figures 2.11, which indicates an immiscible condensing/vaporizing process. Thus, it is very evident that if an adequate number of pseudocomponents for the heavy hydrocarbon fractions is not used, then the mechanisms by which oil is recovered by rich gas injection will be predicted incorrectly, resulting in an overly optimistic prediction of the conditions where miscibility occurs. Our experience with some other injection gas/reservoir oil systems indicate that two pseudocomponents for C_{6+} are adequate to represent condensing/vaporizing processes, while for condensing processes a single C_{6+} pseudocomponent is sufficient.

2.7 Slim-Tube Simulation

Slim-tube simulations were performed for the CO_2 and rich-gas processes described in Sections 2.5 and 2.6. The slim tube has a length of 9.14 m [30 ft], a diameter of 0.64 cm [0.25 in], a porosity of 38 %, and a permeability of 3000 mD. Fluid was injected at a rate of 2.684×10^{-4} m³/day [0.00948 ft³/day], and was produced at a constant pressure.

Figures 2.14 and 2.15 show the curves of oil recovery versus pore volume of gas injected for the CO₂ process at 15000 kPa [2176 psia] and 19000 kPa [2756 psia]. Figures 2.16 and 2.17 show the same curves for the rich-gas process. Excellent agreement was obtained between the few-component and many-component systems.

2.8 Conclusions

1. By choosing appropriately the number of pseudocomponents to model the heavy fractions, and by allowing the critical temperature of the heaviest pseudocomponent to vary with the global composition of a key component, the multiple-contact phase behavior of a 14-component system was modelled accurately using only 4 to 6 components. The pseudoternary diagrams using this approach are virtually identical for the many- and few-component systems.
2. The number of pseudocomponents for the heavy fraction which is required to model the multiple-contact behavior of an injection gas/reservoir oil system depends on whether the process is a vaporizing (liquid-extraction) process or a combined condensing/vaporizing process. For the CO₂/reservoir oil systems studied, which correspond to vaporization (or liquid-extraction) processes, it was found that one pseudocomponent for the heavy fraction was sufficient to model the phase behavior accurately. For rich gas/reservoir oil systems which correspond to condensing/vaporizing processes, it was found that two pseudocomponents for the heavy fraction were required to yield the correct phase behavior.
3. It is important to match the critical point on the pressure-composition diagram if it exists. This is essential for predicting correctly the condensing/vaporizing phenomena.
4. Test runs also confirmed previous observations that the use of one pseudocomponent for C₆₊ yields a condensing process.
5. It is essential that the mechanisms that will occur in a gas-injection process be understood before attempting to select and characterize pseudocomponents. The indiscriminate use of regression may result in a large number of components and yet may still not give the correct phase-behavior mechanisms.
6. The trend of the regressed critical temperature of the heaviest pseudocomponent for a few-component system was very similar for all the cases tested. There was initially a linear decrease with global composition of a key component, and then there was a region where the temperature was constant.

3. K-VALUE CORRELATIONS

3.1 Formulation

In a compositional simulator, two-phase flash calculations with an equation of state are performed in each gridblock at every iteration to determine the oil and gas phase splits, compositions and properties. This involves the solution of the equations describing the equality of component fugacities in the oil and gas phase, i.e.

$$\ln f_{ig}(p, y_{ig}) - \ln f_{io}(p, y_{io}) = 0 \quad i=1, \dots, n_c \quad (3.1)$$

subject to the material-balance constraint

$$z_i = F_g y_{ig} + F_o y_{io} \quad i=1, \dots, n_c \quad (3.2)$$

where

- f_{ij} = fugacity of Component i in Phase j
- y_{ij} = mole fraction of Component i in Phase j
- F_j = mole fraction of Phase j
- z_i = global mole fraction of Phase j
- p = pressure

The fugacities in Equation (3.1) are calculated from an equation of state (EOS). In this investigation the Peng-Robinson EOS (Peng and Robinson, 1976) was used in all examples.

By introducing the K-value defined as

$$K_i \equiv y_{ig} / y_{io} \quad (3.3)$$

Equation (3.1) can be written as follows:

$$\ln K_i + \ln \phi_{ig}(p, y_{ig}) - \ln \phi_{io}(p, y_{io}) = 0 \quad i=1, \dots, n_c \quad (3.4)$$

where $\phi_{ij} = f_{ij} / (y_{ij}p)$ is the fugacity coefficient of Component i in Phase j . An alternate material-balance equation can be derived, i.e.

$$\sum_{i=1}^{n_c} \frac{(K_i - 1)z_i}{1 + F_g(K_i - 1)} = 0 \quad (3.5)$$

Equations (3.4) and (3.5) can be solved for $K_i (i=1, \dots, n_c)$ and F_g . The phase compositions are obtained from

$$y_{io} = z_i / [1 + F_g(K_i - 1)] \quad i=1, \dots, n_c \quad (3.6)$$

$$y_{ig} = K_i y_{io} \quad i=1, \dots, n_c \quad (3.7)$$

Equations (3.4) and (3.5) have to be solved for each gridblock and iteration during the simulation. This results in a substantial amount of computational effort. It is proposed to replace Equation (3.4) by simpler K-value correlations that are consistent with the EOS.

A literature review of K-value correlations was conducted. Most of the K-value correlations available in the literature make use of the concept of convergence pressure. Unfortunately, the calculation of convergence pressure for a reservoir fluid is not well understood, and no general and reliable methods are available or can readily be derived. It was decided to develop the K-value correlations by expanding the fugacity coefficient as a function of pressure in a Taylor series about a reference pressure p^* . The terms of the Taylor series are periodically reevaluated so that the approximate K-values do not differ significantly from the actual K-values calculated from an equation of state. The following expansion was tried:

$$K_i = K_i^* + (\partial K_i / \partial p)^* (p - p^*) \quad (3.8)$$

From Equation (3.4)

$$(\partial \ln K_i / \partial p)^* = (\partial \ln \phi_{io} / \partial p)^* - (\partial \ln \phi_{ig} / \partial p)^* \quad (3.9)$$

Since

$$(\partial \ln K_i / \partial p)^* = \Delta (\partial \ln K_i / \partial K_i)^* (\partial K_i / \partial p)^* = \frac{1}{K_i^*} (\partial K_i / \partial p)^* \quad (3.10)$$

Equation (3.9) becomes

$$(\partial K_i / \partial p)^* = K_i^* [(\partial \ln \phi_{io} / \partial p)^* - (\partial \ln \phi_{ig} / \partial p)^*] \quad (3.11)$$

Equation (3.8) is an expansion of K_i around p^* . It was decided not to include the composition terms because this would necessitate the solution of a system of nonlinear equations for flash calculations that are almost as complex as the equations for actual flash calculations and requires even more storage.

Equation (3.8) can be viewed as a correlation of K_i with respect to pressure. The terms $K_i^* (\partial K_i / \partial p)^*$ and p^* are periodically updated during the simulation to yield approximate K-values which are close to EOS K-values.

3.2 Test Runs With Third SPE Comparative Solution Project

The K-value correlation (3.8) has been implemented in an equation-of-state compositional simulator. Details of the simulator can be found in Collins et al (1986) and Nghiem and Li (1989). The approach was then tested using the Third SPE Comparative Solution Project (Kenyon and Behie, 1987). These SPE Comparative Solution Projects (CSP) are field-scale benchmark problems which were designed to test various aspects of reservoir simulation. The Third CSP deals with the cycling of a gas-condensate reservoir. This CSP was selected as a test run for K-value correlations because it is a sizeable simulation problem (324 gridblocks and 10 components) where compositional effects are important. Indeed, K-values are strongly dependent on pressure and composition during retrograde condensation and revaporization and this problem provides a rigorous test for the proposed approach.

Figure 3.1 shows the discretized reservoir with the well completions. Gas was produced at a constant rate of 175.56×10^3 std m³/day (6.2×10^6 SCF/day). Part of the produced gas was recycled at a constant rate of 133.09×10^3 std m³/day (4.7×10^6 SCF/day).

Simulation runs were performed for 15 years with the EOS flash calculations and the proposed K-value flash calculations. For the K-value runs, actual EOS flash calculations were performed in each gridblock after the first iteration of every timestep to update $K_i^*(\partial K_i / \partial p)^*$ and p^* in Equation (3.8).

Figures 3.2 and 3.3 show the oil production rates and cumulative oil productions for the two runs. Excellent agreements were obtained between the EOS run and the K-value run. Figure 3.4 shows the average reservoir pressure and the oil saturation in Gridblock (7,7,4) which contains the lower completion of the producer. As the reservoir pressure drops below the dew point, oil drops out of the gas condensate and builds up in the gridblock. However, as the pressure further declines the oil revaporizes. There were small discrepancies in the oil saturation during the condensation process between the EOS and K-value runs. Otherwise, the agreement was excellent. The CPU time ratio between K-value run and EOS run is 0.82 which corresponds to a savings of 18%.

4. GENERAL FLASH CALCULATIONS

4.1 Outline

A flash-calculation procedure called "general flash calculations" is described and compared to the current approach for flash calculations with stability tests. Calculations for two-phase systems are elaborated first and extensions to systems with three or more phases follow.

To highlight the differences between the current approach for flash calculations and the approach investigated here, a review of the current approach is given below.

4.2 Current Two-Phase Flash Calculations with Stability Tests

As described in Section 2, flash calculations with an EOS involve the solution of the following equations

$$g_i \equiv \ln K_i + \ln \phi_{ig} - \ln \phi_{io} = 0 \quad i=1, \dots, n_c \quad (4.1)$$

$$h \equiv \sum_{i=1}^{n_c} \frac{(K_i - 1)z_i}{1 + F_g(K_i - 1)} = 0 \quad (4.2)$$

The above equations can be solved with Newton's method. A more efficient method was suggested by Nghiem and Heidemann (1982) and Nghiem and Li (1984). Their method called QNSS (for Quasi-Newton Successive Substitution) is as follows. First define:

$$\xi_i \equiv \ln K_i \quad (4.3)$$

$$\Delta \xi^{(k)} \equiv \xi^{(k+1)} - \xi^{(k)} \quad (4.4)$$

where $\xi^{(k)}$ is the k -th iterate of ξ . The QNSS iteration corresponds to

$$\Delta \xi^{(k)} = -\sigma^{(k)} g^{(k)} \quad (4.5a)$$

$$\sigma^{(k)} = - \left[\Delta \xi^{(k-1)T} g^{(k-1)} / \Delta \xi^{(k-1)T} \Delta g^{(k-1)} \right] \sigma^{(k-1)} \quad (4.5b)$$

$$\sigma^{(0)} = 1 \quad (4.5c)$$

where the superscript T denotes the transpose. After each iteration, Equation (4.2) is solved for F_g , the mole fraction of the gas phase. For two-phase systems, the value of F_g is between zero and unity.

The major complications in performing two-phase flash calculations are the initiation of the calculations and the detection of single-phase regions. These can be resolved by performing a stability test based on an analysis of the Gibbs energy surface as described in Michelsen (1982) and Nghiem and Li (1984). A stability test of a mixture of composition x_i at given p and T consists of solving the following equation

$$\ln Y_i + \ln \phi_i(y) - \ln x_i - \ln \phi_i(x) = 0 \quad i=1, \dots, n_c \quad (4.6)$$

$$y_i = Y_i / \sum_{j=1}^{n_c} Y_j \quad (4.7)$$

for Y_i . The mixture x_i is stable (single-phase) if the resulting Y_i 's satisfy the inequality

$$\sum_{j=1}^{n_c} Y_j \leq 1 \quad (4.8)$$

If on the other hand $\sum_{j=1}^{n_c} Y_j > 1$, the mixture x_i is unstable and will split into two phases. Two-phase flash calculations can be initiated with an initial guess

$$K_i^{(0)} = Y_i / x_i \quad (4.9)$$

It has been demonstrated that the above values provide excellent guesses for flash calculations.

To initiate the stability test calculations, the following set of $Y_i^{(0)}$ are recommended

$$(a) \quad Y_i^{(0)} = K_i^w x_i \quad (4.10a)$$

$$(b) \quad Y_i^{(0)} = x_i / K_i^w \quad (4.10b)$$

$$(c) \quad Y_i^{(0)} = \phi_i(x) \quad (4.10c)$$

where K_i^w are Wilson's K-values given by

$$K_i^w = \frac{P}{P_{ci}} \exp[5.373(1 + \omega_i)(1 - T_{ci}/T)] \quad (4.11)$$

Often, two of the sets of initial guesses in (4.10) converge to the trivial solution (i.e. $K_i=1$ for all i) while the remaining set gives the desired solution.

4.3 General Two-Phase Flash Calculations

In this technique, Equations (4.1) and (4.2) are always used, irrespective of whether the system is single-phase or two-phase. No stability testing is applied to determine single-phase regions or to generate initial K-values for two-phase calculations.

In the two-phase regions, the solution yields a value for F_g between zero and unity while a negative value for F_g indicates a single-phase oil and a value for F_g greater than unity indicates a single-phase gas. Convergence to the trivial solution, i.e. all K_i 's are equal to unity, indicates a

supercritical system. This concept of this technique was briefly mentioned in Li and Nghiem (1982) but no research was pursued because of the success of the standard flash calculation methods. Recently, Whitson and Michelsen (1989) pointed out some advantages of the concept. One obvious advantage is the simplicity of the programming method because of the elimination of the stability test calculations. It was proposed to also investigate the concept for EOS flash calculations and to compare it with the standard approach for flash calculations which includes stability testing.

4.4 Two-Phase Examples

Table 4.1 shows the composition of Reservoir Oil A and Reservoir Gas B which were used to demonstrate the general flash procedure.

For Oil A, calculations were performed at 36°C and increasing pressures as indicated in Table 4.2. Table 4.2 reports the calculated gas molar fraction F_g , the number of calls to the subroutine EOS to calculate densities and fugacities from pressure and compositions, and the initial guesses for the calculations. The number of calls to EOS is a good indication of the computational effort involved. It was found that for two-phase systems, both the standard calculations and the general calculations performed similarly. In the single-phase regions close to the saturation pressure, the general calculations require less computational effort. However, in the supercritical regions, the standard calculations are more efficient.

Table 4.3 shows the same calculations performed with Gas B. The same conclusions as in the case of Oil A can be drawn.

Although general flash calculations do not always entail less computation, they provide a criterion to identify a single-phase system as a gas, an oil or a supercritical fluid.

Simulation of gas-injection processes normally requires two-phase (oil/gas) calculations. The presence of the water phase may necessitate three-phase flash calculations because of the gas solubility in water. However, this solubility can be modelled accurately with Henry's law (Li and Nghiem, 1986) rather than with an equation of state. Recently, Agarwal et al (1990) described a procedure for taking into account of gas solubilities in a compositional simulator without the requirement of a three-phase flash-calculation procedure.

In CO₂ flooding, three hydrocarbon phases (oil-rich liquid/CO₂-rich liquid/gas) may be encountered (Stalkup, 1984, p. 9). With the presence of water and the possibility of asphaltene precipitation, more than three phases may coexist. A few algorithms for four-phase flash calculations have been described in the literature (Risnes and Dalen, 1984; Enrick et al, 1987) but no calculations with more than four phases have been reported.

For completeness, it was decided to compare the general flash-calculation algorithm and the flash-calculation algorithm with stability tests for systems with more than three phases. Using the experience gained in developing the above algorithms, procedures were constructed for systems with an arbitrary number of phases. This would allow the study any fluid systems with complex phase behavior.

4.5 Extension to Multi-Phase Systems

Three-phase flash calculations with stability tests can be performed in a stagewise procedure as illustrated in Figure 4.1 (Nghiem and Li, 1984, 1989). The general flash-calculation approach can be

extended to three-phase system in a similar fashion as depicted in Figure 4.2. Note that all stability tests in Figure 4.1 have been replaced by the testing of the sign of F_j , $j=o,q,g$, where the subscripts o and q denote the two liquid phases.

Calculations performed on a variety of three-phase systems revealed that the general three-phase flash calculations were not as robust as the calculations with stability tests. The general calculations have the tendency to converge to a trivial solution (i.e. two phases having the same compositions) and cannot proceed once one of the phases disappears during iterations, which is quite common in three-phase calculations.

Because of the robustness of the calculations with stability tests, it was decided to extend the techniques to systems with any number of phases. This results in the algorithm illustrated in Figure 4.3.

Calculations were carried out with the 6-component system shown in Table 4.4 which is based on a 4-component system communicated to us by Dr. R.A. Heidemann of the University of Calgary. This system splits into 6 phases as shown in Table 4.4. The Soave-Redlich-Kwong EOS (Soave, 1972) was used in the predictions.

4.6 Conclusions

A flash-calculation procedure called "general flash calculations" has been developed. This procedure does not require stability-test calculations as in the current technique for flash calculations. The calculation procedure has been implemented in a compositional simulator.

For two-phase systems, test runs showed that the proposed procedure is competitive in robustness and performance with the current technique, with a simpler code. However, for systems with more than two phases, the current technique is more robust.

The technique with stability tests has been extended to systems with any number of phases. A six-phase separation was successfully predicted.

5. OPTIMIZATION OF TIMESTEP SIZE IN COMPOSITIONAL SIMULATION

5.1 Outline

Usually, the fewer timesteps taken in a reservoir simulation, the faster the simulation can be performed. However, three effects set an upper limit upon the timestep size:

- (1) Accuracy: in most finite difference schemes used in reservoir simulation, the error in the simulated quantities increases linearly with the timestep size;
- (2) Computational effort: when the timestep is too large, more Newtonian iterations may be required; the total computational time is then likely to increase even if the number of timesteps decreases;
- (3) Stability: when explicit discretizations are used for reservoir gridblocks, the solution becomes unstable if the timestep exceeds a certain limit.

Traditionally, compositional simulators have selected timestep sizes based on considerations (1) and (2). Stability has been maintained either by doing fully implicit simulations, or by setting a sufficiently small maximum timestep size (if some gridblocks are constrained to be explicit), or by switching blocks from explicit to implicit as needed to maintain stability for a given timestep size. Recently, a method has been developed (Grabenstetter et al, 1991) for the practical detection of instability in compositional simulations. In this task, the method is applied to consider stability directly in timestep size selection for compositional reservoir simulations.

This section is organized as follows. The problem is introduced in Section 5.2, and the two approaches under investigation, the adaptive implicit and fixed map approaches, are described. The adaptive implicit approach is developed in Section 5.3, and the fixed map approach in 5.4. An analysis of computation time usage in compositional simulation, which was needed for the adaptive implicit approach, is presented in Section 5.5. Results are presented in Section 5.6 and discussed in Section 5.7.

5.2 Background

In finite difference computational schemes for oil or gas reservoir simulation, the reservoir is divided into gridblocks. At a given timestep in a simulation a gridblock can be treated in either of two ways:

- (1) Explicit discretization: In the $n+1$ -st timestep, variable values at the n -th time level (the old level) are used to compute variable values at the $n+1$ -st time level (the new level) by a direct (non-iterative) calculation;
- (2) Implicit discretization: In the $n+1$ -st timestep, variable values at the new time level are used to compute the final variable values at the new time level by an iterative scheme, usually Newton's method.

In practice the pressure variable in all gridblocks is treated implicitly, and hence some iteration is always necessary, but in general the fewer implicit gridblocks there are, the less CPU time is required to complete the timestep.

However, if the timestep is too large, the explicit discretization is unstable, and perturbations in the solution grow in succeeding timesteps. The solution then eventually becomes extremely inaccurate. This implicit discretization is stable however large the timestep, although for very large timesteps the implicit discretization is likely to be inaccurate, even though stable.

There have been two general approaches to the designation of gridblocks as implicit or explicit in reservoir simulation:

- (1) Fixed map method: Blocks are initially designated as implicit or explicit and retain this designation throughout the simulation. The initial designation is arbitrary, but two particular choices are widely used:
 - (a) Fully implicit map: All variables in all gridblocks are treated implicitly; stability is then not a concern in timestep selection.
 - (b) Explicit map: In non-well gridblocks all variables except pressure are treated explicitly. In some implementations well blocks also follow this pattern; in others well blocks are fully implicit. Stability is maintained by setting a sufficiently small maximum timestep size.
- (2) Adaptive implicit method: A test is applied at the start of a timestep to decide which gridblocks must be implicit in order to maintain stability, given a preselected timestep size. Blocks are then switched as necessary.

The instability detection method (Grabenstetter et al, 1991) used here is based on the Courant-Friedrichs-Lewy (CFL) test for the stability of explicit discretizations of linear systems of hyperbolic partial differential equations. Currently this test is used as described in (2) to switch gridblock designations. Two new applications of the CFL test to consider stability in the timestep selection algorithm are under investigation:

- (1) In adaptive implicit simulations, the preselected timestep size may be so large that many blocks must switch to implicit. This may increase the CPU time required per iteration so much that the advantage in reducing the number of timesteps is lost. The CFL test allows estimation of the CPU time reduction resulting from using a shorter timestep.
- (2) In fixed map simulations containing explicit blocks, the maximum timestep size is set by making trial simulations and usually remains fixed throughout the simulation. The CFL test allows a timestep size to be proposed as in an adaptive implicit simulation, and cut as needed to maintain stability. This offers the possibility of reducing the number of timesteps without reducing the accuracy of the results. It also eliminates the need for trial runs to find the maximum allowable timestep size.

The following two sections describe these approaches in detail.

5.3 Stability Based Timestep Selection in Adaptive Implicit Compositional Simulation

One measure of the computational efficiency of a reservoir simulation is the ratio of the CPU time needed for the simulation to the length of the simulated time interval,

$$r = \text{CPU} / (t_f - t_i) \quad (5.1)$$

The smaller r is, the more computationally efficient the simulation is. This measure is valid for comparing two simulations only if the same scenario is run on the same computer.

The approach taken here for timestep selection is to attempt to reduce r in each timestep by considering stability effects.

The $n+1$ -st timestep of a simulation has initial time t^n . A proposed timestep length Δt_p^{n+1} is selected for this timestep based on considerations not directly involving stability, such as maintaining changes in variable values at prescribed levels.

The CFL criterion can be applied to determine which of the gridblocks must be implicit if the timestep size is to be Δt_p^{n+1} . It can also determine, at a negligible additional expense, which blocks must be implicit if some other specified timestep length is used. Consider an alternate timestep length $\alpha \Delta t_p^{n+1}$, which differs from Δt_p^{n+1} by the multiplicative factor α . The case of interest here is for $0 < \alpha < 1$, that is when the timestep is shortened by the factor α .

Analogously to equation (5.1), consider a ratio specific to the $n+1$ -st timestep, expressed as a function of the timestep length,

$$r^{n+1}(\Delta t) = \text{CPU}(\Delta t) / \Delta t; \quad (5.2)$$

here $\Delta t = t^{n+1} - t^n$ and $\text{CPU}(\Delta t)$ is the computation time necessary for the $n+1$ -st step when Δt is the step length. A shift from step length Δt_p^{n+1} to $\alpha \Delta t_p^{n+1}$ is advantageous if

$$r^{n+1}(\alpha \Delta t_p^{n+1}) < r^{n+1}(\Delta t_p^{n+1}). \quad (5.3)$$

We denote

$$\text{CPU}(\alpha \Delta t_p^{n+1}) = \text{CPU}(\Delta t_p^{n+1}) - \Delta \text{CPU}(\alpha)$$

Reducing Δt should reduce $\text{CPU}(\Delta t)$ if the number of implicit blocks in the reservoir is decreased and if the number of Newtonian iterations needed for the timestep does not increase when the timestep is shortened.

With this notation, condition (5.3) becomes

$$\frac{\text{CPU}(\Delta t_p^{n+1}) - \Delta \text{CPU}(\alpha)}{\alpha \Delta t_p^{n+1}} < \frac{\text{CPU}(\Delta t_p^{n+1})}{\Delta t_p^{n+1}},$$

which is equivalent to

$$\frac{\Delta \text{CPU}(\alpha)}{\text{CPU}(\Delta t_p^{n+1})} > 1 - \alpha. \quad (5.4)$$

Thus, for example, a cut to a timestep 90% as long as the proposed value ($\alpha=0.9$) increases the computation efficiency if the CPU time necessary for the timestep is reduced by more than 10%.

The parameter α is adjustable; for a given value of α the test (5.4) can be computed if $\text{CPU}(\Delta t_p^{n+1})$ and $\Delta\text{CPU}(\alpha)$, or at least their ratio, can be estimated. We assume that the number of Newtonian iterations needed for the timestep is unchanged by the timestep cut so that $\Delta\text{CPU}/\text{CPU}$ for the whole timestep is well estimated by the same ratio for a single Newtonian iteration. The estimation of $\Delta\text{CPU}/\text{CPU}$ then requires an examination of how the implicit/explicit designations of the gridblocks depend on the timestep length and in turn how the CPU time needed for a timestep depends upon the block designations.

In an adaptive implicit compositional simulation using the CFL criterion, magnitudes of component front velocities are computed in those gridblocks tested in the current timestep. Usually blocks in the following three categories are tested:

- (1) Implicit non-well blocks;
- (2) Explicit neighbors of implicit blocks;
- (3) Blocks in which a gas or water phase first became mobile in the last timestep.

We denote the largest front velocity magnitude in gridblock i as v_i . In addition a discretization velocity u_i is computed for block i . In the simple case of a one-dimensional reservoir

$$u_i = \Delta x_i / \Delta t,$$

where Δx_i is the length of the i -th gridblock. For multiple spatial dimensions the numerator is a more complicated function of gridblock dimensions, but u_i is always inversely proportional to the timestep length Δt . Block i is stable when discretized explicitly if

$$v_i < u_i. \quad (5.5)$$

The computation of v_i does not depend on Δt ; hence if the timestep is cut to $\alpha\Delta t$, then block i is stable if

$$v_i < u_i / \alpha. \quad (5.6)$$

The discretizations of all gridblocks are recorded as a vector d with components d_i , $i=1, \dots, n_b$; if block i is explicit $d_i = 0$, if implicit, $d_i = 1$. Here n_b is the number of gridblocks. Using (5.5) and (5.6), $d(\Delta t)$ and $d(\alpha\Delta t)$ can be computed with only a single computation of front velocities.

The details of estimating $\Delta\text{CPU}/\text{CPU}$ once $d(\alpha\Delta t_p^{n+1})$ and $d(\Delta t_p^{n+1})$ are known are given in Section 5.5. The algorithm for selection of the $n+1$ -st timestep length Δt^{n+1} which results is as follows:

- (1) Choose $0 < \alpha < 1$;
- (2) Generate Δt_p^{n+1} without taking stability into account;
- (3) Determine $d(\Delta t_p^{n+1})$ and $d(\alpha\Delta t_p^{n+1})$;
- (4) Estimate $c = \Delta\text{CPU}(\alpha) / \text{CPU}(\Delta t_p^{n+1})$;

- (5) If $c > 1 - \alpha$, then $\Delta t^{n+1} = \alpha \Delta t_p^{n+1}$, else $\Delta t^{n+1} = \Delta t_p^{n+1}$.

This algorithm was coded; results are presented in Section 5.6.

5.4 Fixed Map Timestep Selection For Compositional Simulation

Consider a fixed map simulation in which at least one block is designated as explicit (otherwise no stability test is needed). As before we take Δt_p^{n+1} to be proposed steplength for the $n+1$ -st timestep selected without regard to stability.

Stability testing will not be applied to all explicit blocks, but only to the following subset:

- (1) All explicit blocks neighboring implicit blocks;
- (2) All explicit blocks in which a gas or water phase first became mobile in the last timestep.

If, for example, explicit block i is tested and

$$v_i \leq u_i(\Delta t_p^{n+1})$$

then block i is stable with timestep length Δt_p^{n+1} ; if however

$$\beta_i \equiv v_i / u_i(\Delta t_p^{n+1}) > 1 \tag{5.7}$$

then block i is stable only for timesteps of length $\Delta t_p^{n+1} / \beta_i$ or less.

The algorithm for stability-based selection of Δt^{n+1} which results from the above considerations is as follows:

- (1) Based on the fixed map, determine a set E of indices of explicit gridblocks to be tested;
- (2) Calculate Δt_p^{n+1} based on considerations other than stability
- (3) Compute β_i , $i \in E$, and $\beta = \max_{i \in E} \beta_i$
- (4) If $\beta \leq 1.0$, then $\Delta t^{n+1} = \Delta t_p^{n+1}$, else set $\Delta t^{n+1} = \Delta t_p^{n+1} / \beta$

Results of tests of this algorithm are presented in Section 5.6.

5.5 Prediction of CPU Times for One Newtonian Iteration of Adaptive Implicit Compositional Simulation

There are four computational procedures which together account for at least 90% of the CPU time needed in a compositional simulation:

- (1) Building the Jacobian matrix of the reservoir equations at each Newtonian iteration;
- (2) Solving the resulting linear system of equations at each iteration;

- (3) Updating the physical property values in all gridblocks using a thermodynamic equation of state at each iteration;
- (4) Checking the stability of a subset of the gridblocks, once per timestep.

The CPU time required per iteration can be estimated if estimates are available for these four procedures individually (for procedure (4), the average number of iterations per timestep must also be known).

The CPU times for these procedures depend strongly on the following parameters:

n_c :	:	the number of hydrocarbon components used in the simulation;
n_{eq}	:	the number of reservoir equations per gridblock, usually n_c+2 ;
$n_{con}(i)$	:	the number of other gridblocks connected to block i ;
$d(i)$	:	discretization (implicit or explicit) of block i ;
F_{imp}	:	the fraction of gridblocks which are implicit;
$n_{ph}(i)$	:	the number of hydrocarbon phases present in gridblock i ;
n_b	:	the number of gridblocks in the reservoir.

The actual CPU times for the four procedures depend strongly upon the characteristics of the computing machine used, but the ratios $\Delta CPU/CPU$ should depend much less strongly on machine type. The ratios probably depend somewhat on machine architecture; for example, a reduced-instruction-set (RISC) machine may yield $\Delta CPU/CPU$ ratios differing systematically from those obtained on machines with a complex-instruction-set architecture. Despite this, it is not expected that machine differences affect $\Delta CPU/CPU$ strongly enough to alter frequently the decision to cut a timestep or not.

The CPU time estimates for the four principal procedures were found to be as follows:

- Jacobian building: The CPU time needed for one Newtonian iteration of this procedure is well approximated as the sum of the CPU times for the individual blocks. The CPU time for block i depends strongly on $n_{ph}(i)$, $d(i)$, $n_{con}(i)$, and n_{eq} . Block CPU times for a set of primary production simulations were fit by linear regression to polynomials in n_{eq} and $n_{con}(i)$. In these simulations the water saturation was fixed at zero; hence $n_{eq} = n_c + 1$ here. The predictive function which resulted has the form

$$CPU(i) = a n_{con}(i) + b$$

where a and b are quadratic functions of n_{eq} . Four different pairs of quadratic expressions for a and b were found, for implicit or explicit blocks containing one or two hydrocarbon phases.

- Linear system solution: The CPU time needed for one Newtonian iteration of this procedure depends strongly upon n_{eq} , n_b , and F_{imp} . The predictive function has the form

$$CPU = aF_{imp}^2 + bF_{imp} + c,$$

where a is a cubic, b a quadratic, and c a linear function of n_{eq} . The expansion coefficients for a , b , and c in turn depend on n_b .

- Property updates: The CPU time for one Newtonian iteration of this procedure is well approximated as a block sum. The CPU time for block i depends strongly on n_c , $d(i)$, and $n_{ph}(i)$. The predictive function has the form

$$CPU(i) = an_c^2 + bn_c + c,$$

with four different triples a , b , c for implicit or explicit blocks containing one or two hydrocarbon phases.

- Stability testing: The CPU time for this procedure in one timestep is well approximated as a block sum. For block i the CPU time depends strongly on n_{eq} , $n_{ph}(i)$, $d(i)$, and $n_{con}(i)$.

The predictive function has the form

$$CPU(i) = a n_{con}(i) + b,$$

where a and b are quadratic functions of n_{eq} . There are four pairs of quadratic expressions for a and b , for implicit and explicit blocks containing one or two hydrocarbon phases. $CPU(i)$ is then divided by the average number of iterations per timestep.

The predictive functions described above were coded and used in the tests reported in the next section.

5.6 Test Results

The approaches described in Sections 5.3 and 5.4 were tested on two problems: the Third SPE Comparative Solution Project (SPE 3) problem (Kenyon and Behie, 1987), and the Fifth SPE Comparative Solution Project (SPE 5) problem (Killough and Kossack, 1987). The SPE 3 problem was summarized in Section 3. The SPE 5 problem is a miscible flood simulation involving two-year water-alternating-gas (WAG) injection cycles. The fluid is modelled with 6 hydrocarbon components and the reservoir has 147 gridblocks. Simulation continues until water breaks through at the producing well, which occurs at about 18 years of simulation time.

Results for the adaptive implicit approach described in Section 5.3 are presented in Table 5.1. For the SPE 5 problem, the maximal CPU saving of about 4% is obtained with $\alpha = 0.90$. For the SPE 3 problem, the maximal CPU saving is about 1% and is obtained with $\alpha = 0.95$. Since CPU times for a given run are reproducible only to within 1%, it is questionable whether the actual computational effort is reduced for any value of α in the SPE 3 problem.

Test results for the fixed map timestep selection algorithm introduced in Section 5.4 are presented in Table 5.2. For both test problems, the total CPU time is increased (by a factor of roughly 1.5) rather than decreased by applying the stability based algorithm. The timesteps are typically shorter when this algorithm is used than with the traditional approach.

5.7 Discussion

The results show that the algorithm of Section 5.3 does not result in a significant reduction in CPU time compared to the traditional approach and that the algorithm of Section 5.4 actually increases the CPU time compared to the traditional approach.

For the adaptive implicit timestep selection algorithm (Section 5.3), the reason for this failure is apparently that in typical simulations little or no saving can be achieved by reducing timesteps. This can be attributed to the fact that adaptive-implicit simulation with CFL switching criteria yield already near-optimal run time. Indeed, test runs with the latter technique reported in Grabenstetter et al (1991) shows substantial savings compared to other techniques.

For the fixed map algorithm (Section 5.4) the reasons for the failure are less clear. It appears that the traditional fully explicit simulation maintains some blocks well above the CFL stability limit without incurring unacceptably large errors.

6. FIELD-SCALE TEST RUNS

The techniques for optimal pseudocomponent representation (Section 2) and K-value correlations (Section 3) are tested in the following using actual field data. The reservoir has 2002 gridblocks (13x14x11) and 29 wells as shown in Figure 6.1. Both gas-injection runs and black-oil type runs were performed.

For the gas-injection runs, the CO₂/reservoir oil system of Sigmund et al (1979) described in Section 2.5 was used. Three runs were performed: 1) 14 components with EOS flash calculations; 2) 4 components with EOS flash calculations; 3) 4 components with K-values correlations. The purpose of the above runs is to find out the improvements obtained with the different techniques developed in this project

For the black-oil type runs, the black-oil data from the Fifth SPE Comparative Solution Project (Killough and Kossack, 1987) were converted to two pseudocomponents for the Peng-Robinson equation of state. Compositional simulation runs were then performed to compare results and run times with an actual black-oil simulator. The purpose of these runs is to compare an improved compositional simulator with two pseudocomponents and K-value correlations to a black-oil simulator for typical black-oil problems.

6.1 CO₂ Injection Process

Figures 6.2 to 6.6 summarize the field-scale simulation results obtained with 14 components and 4 components using EOS flash calculations. The amount of oil recovered and the oil rate are in excellent agreement for the 14 component and the 4 component systems. The average reservoir pressure is also in good agreement. The producing gas-oil ratio and water cut are in good agreement at early times. Some discrepancies occur late in the run, but these are not significant because the oil rate is small at the end of the run. These discrepancies were caused by differences in producing well shut-off times due to violations of bottomhole pressure and GOR constraints. The discrepancies however, were not reflected in the oil recovery curves where there was excellent agreement between the results for 14 and 4 components. These results demonstrate again that the pseudocomponent characterization technique described in Section 2 is very adequate in reducing the number of components. Runs with 4 components and K-value correlations show results which are almost identical to the 4-component runs with EOS flash calculations. The run-time ratios between the different runs are shown in Table 6.1. The use of 4 components instead of 14 components yields a speed up factor of more than 5.5. Only a small speed-up was obtained between EOS flash calculations and K-value correlations. An examination shows that this is caused by the small number of components used. K-value correlations give greater savings with higher numbers of components. Test runs with 10 components in Section 3.2 yielded a savings of 18% while runs with 4 components above yielded a savings of only 4%.

6.2 Black-Oil Type Run

Figures 6.7 to 6.10 show the results obtained with a compositional simulator with two pseudocomponents and with an actual black-oil simulator. For the compositional simulation runs, both EOS flash calculations and K-value correlations were used. Excellent agreement was obtained for oil rates, cumulative oil production, average reservoir pressure and water cut. Table 6.1 shows the run-time ratios for the different simulations. It was observed that although the number of components has been reduced to two, compositional simulation is still much more expensive than black-oil simulation. A close examination of the runs shows that high the cost of compositional

simulation is caused by the evaluations of the logarithms and exponentiations required by the EOS whereas a black-oil simulator requires only table look-up. In the case of K-value correlations, the EOS is still used to calculate densities and to generate periodically the parameters of the correlations (see Section 3.1).

6.3 Conclusions

The above field-scale test runs show that the reduction of the number of components has the largest impact on run times in compositional simulation. The technique developed in Section 2 allows a drastic reduction in run time without any significant loss in accuracy.

The K-value correlations are valuable when a large number of components are used as in the case of the Third Comparative Solution Project in Section 3.2. When the number components is small, only a small saving was obtained.

7. CONCLUSIONS

This report described techniques for speeding up EOS compositional simulators so that they can be used routinely in field-scale simulation. The techniques include:

1. The reduction of the number of components through the optimal representation of the heavy fractions.
2. The development of K-value correlations consistent with the equation of state.
3. The development of a general flash calculation algorithm that simplifies the detection of single-phase regions.
4. The development of a timestep selection algorithm that optimizes the number of implicit gridblocks.

The following conclusions are obtained:

1. A technique for optimal representation of the heavy fractions was developed. It allows a drastic reduction in the number of components without significant loss in accuracy. It has the largest impact in run-time reduction.
2. A K-value correlation based on the expansion of the EOS was developed. It is valuable when the number of components is large (around ten). For systems with few components (four or less), the savings is small (around 4%).
3. The performance of the general flash calculations is comparable to the current flash calculations with stability tests. However, the coding is much simpler. A flash calculation algorithm for systems with any number of phases was also developed.
4. The timestep selection based on the optimal number of implicit gridblock yields only marginal reduction in run times. This can be attributed to the fact that adaptive-implicit simulation with CFL switching criteria yield already near-optimal run time. Indeed, test runs with the latter technique reported in Grabenstetter et al (1991) shows substantial savings compared to other techniques.

8. ACKNOWLEDGEMENTS

This research was supported by Canada Centre for Mineral Energy Technology (CANMET) and by the Members of the Computer Modelling Group.

9. NOMENCLATURE

f_{ij}	fugacity of Component i in Phase j (j=o,g,q)
F_j	mole fraction of Phase j
K_i	K-value of Component i
g_i	defined in Equation (4.1)
h	defined in Equation (4.2)
p	pressure
r	ratio of CPU time over simulation time
T	temperature
T_c	critical temperature
u	velocity
v	velocity
y_{ij}	mole fraction of Component i in Phase j
z_i	global mole fraction of Component i

Greek

α	timestep reduction factor
Δt	timestep size
ξ_i	$= \ln(K_i)$
ϕ_{ij}	fugacity coefficient of Component i in Phase j
σ	step size in QNSS technique
ω_i	acentric factor of Component i

Subscript

g	gas
o	oil
q	second hydrocarbon liquid phase
w	water

Superscript

(k)	iteration level
n	old time step
$n+1$	new time step

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TABLE 2.1
Saturation Pressure Experimental Data of Sigmund et al (1979) Fluids
(T = 96.6°C)

Component or property	Recombined reservoir fluid	Recombined reservoir fluid + CO ₂			
	No. 1	No. 2	No. 3	No. 4	No. 5
CO ₂ (mole %)	1.64	18.45	37.03	56.79	77.74
N ₂	2.18	1.81	1.40	0.96	0.49
C ₁	28.99	24.03	18.55	12.73	6.57
C ₂	7.97	6.61	5.10	3.50	1.80
C ₃	7.15	5.93	4.58	3.14	1.62
i-C ₄	1.21	1.00	0.77	0.53	0.27
n-C ₄	3.54	2.94	2.27	1.56	0.80
i-C ₅	2.00	1.66	1.28	0.88	0.45
n-C ₅	2.12	1.76	1.36	0.93	0.48
C ₆₊	43.20	35.81	27.66	18.98	9.78
C ₆₊ density at 15.6°C	0.8358	0.8358	0.8358	0.8358	0.8358
C ₆₊ molecular weight	178.47	178.47	178.47	178.47	178.47
Bubble point pressure (kPa)	15858	18650	20305	24235	41368

Reservoir Fluid Analysis of C₆₊ Fraction to C₃₀₊

Component	Mole %	Component	Mole %	Component	Mole %
C ₆	1.94	C ₁₅	1.35	C ₂₃	0.45
C ₇	7.01	C ₁₆	0.85	C ₂₄	0.23
C ₈	8.06	C ₁₇	0.79	C ₂₅	0.22
C ₉	5.54	C ₁₈	0.58	C ₂₆	0.22
C ₁₀	4.37	C ₁₉	0.47	C ₂₇	0.22
C ₁₁	2.94	C ₂₀	0.41	C ₂₈	0.22
C ₁₂	2.23	C ₂₁	0.33	C ₂₉	0.22
C ₁₃	2.10	C ₂₂	0.32	C ₃₀₊	0.83
C ₁₄	1.30				

TABLE 2.2
Representation of Sigmund et al (1979) Reservoir Oil

14 Components		4 Components	
Comp.	mole %	Comp.	mole %
CO ₂	1.64	CO ₂	1.64
N ₂	2.18	C ₁ -N ₂	31.17
C ₁	28.99	C ₂ -C ₅	23.99
C ₂	7.97	C ₆₊	43.2
C ₃	7.15		
iC ₄	1.21		
nC ₄	3.54		
iC ₅	2.00		
nC ₅	2.12		
C ₆ -C ₉	12.24		
C ₁₀ -C ₁₂	13.36		
C ₁₃ -C ₁₆	8.44		
C ₁₇ -C ₂₀	4.68		
C ₂₁₊	4.47		

TABLE 2.3
Representation of Sigmund et al (1979)
Reservoir Oil with Rich Gas Injection

Component	14 Components		Component	6 Components	
	Oil Mole %	Solvent Mole %		Oil Mole %	Solvent Mole %
CO ₂	1.64		C ₂ -C ₃ (Solvent)	0.0	70
N ₂	2.18		CO ₂ -N ₂	3.82	
C ₁	28.99	30	C ₁	28.99	30
C ₂	7.97	40	C ₂ -C ₅	23.99	
C ₃	7.13	30	C ₆ -C ₁₂	25.60	
iC ₄	1.21		C ₁₃₊	17.60	
nC ₄	3.54				
iC ₅	2.00				
nC ₅	2.12				
C ₆ -C ₉	12.24				
C ₁₀ -C ₁₂	13.36				
C ₁₃ -C ₁₆	8.44				
C ₁₇ -C ₂₀	4.68				
C ₂₁₊	4.47				

TABLE 4.1
Composition of Reservoir Oil A and Reservoir Gas B

Oil A		Gas B	
Component	Mole %	Component	Mole %
N ₂	0.34375	C ₁ +N ₂	77.0000
CO ₂	3.06249	C ₂ +CO ₂	10.0000
CH ₄	43.69791	C ₃ +C ₄	6.0000
C ₂ H ₆	9.08333	C ₅	1.0000
C ₃ H ₈	6.16666	C ₆ -C ₁₂	4.9000
iC ₄	1.39583	C ₁₃ -C ₂₁	1.0000
nC ₄	2.91666	C ₂₂ +	0.1000
iC ₅	1.26041		
nC ₅	1.51041		
C ₆ -C ₁₂	19.88541		
C ₁₃ -C ₂₁	10.67708		
C ₂₂ +	0.00001		

TABLE 4.2
Comparison of Calculations for Oil A (T = 36.0°C)

Pressure (kPa)	Standard Flash Calculations With Stability Tests			General Flash Calculations		
	F_g	No. of Calls to EOS	Initial Guesses	F_g	No. of Calls to EOS	Initial Guesses
101	0.9964	8	Eqn (4.10a)	0.9964	8	Eqn (4.10a)
1000	0.9550	8	id.	0.9550	8	id.
5000	0.7083	10	id.	0.7083	10	id.
10000	0.3806	12	id.	0.3806	12	id.
15000	0.1101	18	id.	0.1101	18	id.
17300	0.0035	30	id.	0.0035	18	id.
17400	0.0000	22	id.	-0.0010	18	id.
17600	0.0000	22	Eqns (4.10a+b)	-0.0100	18	id.
18000	0.0000	23	id.	-0.0280	18	id.
20000	0.0000	27	id.	-0.1187	20	id.
25000	0.0000	28	id.	-0.3970	34	id.
35000	0.0000	24	id.	*	73	Eqns (4.10a+c)

* Convergence to the trivial solution with all K_i 's equal to unity.

TABLE 4.3
Comparison of Calculations for Gas B (T = 92.2°C)

Pressure (kPa)	Standard Flash Calculations With Stability Tests			General Flash Calculations		
	F_g	No. of Calls to EOS	Initial Guesses	F_g	No. of Calls to EOS	Initial Guesses
101	0.9999	8	Eqn (4.10a)	0.9999	8	Eqn (4.10a)
1000	0.9970	8	id.	0.9970	8	id.
10000	0.9464	12	id.	0.9464	12	id.
20000	0.8959	18	id.	0.8959	18	id.
30000	0.9295	40	id.	0.9295	40	id.
37434	1.0000	52	Eqns (4.10a+b)	1.0000	62	id.
37500	1.0000	51	id.	1.0000	72	Eqns (4.10a+c)
38000	1.0000	58	id.	*	49	id.
40000	1.0000	54	id.	*	43	id.
50000	1.0000	32	id.	*	21	id.

* Convergence to the trivial solution with all K_i 's equal to unity.

TABLE 4.4
Six-Phase Multicomponent System

Component	Feed	Mole Percent					
		Phase 1	Phase 2	Phase 3	Phase 4	Phase 5	Phase 6
CO ₂	5.6273	0.0001	6.1355	6.3542	4.9924	4.7943	1.8711
H ₂ S	40.8168	0.0017	68.3731	35.3731	16.4825	16.4485	3.3112
C ₁	49.0196	0.0000	23.6628	53.8053	39.5526	77.4612	94.8122
C ₆	2.5754	0.0000	1.8094	3.8591	0.5887	1.2952	0.0055
C ₄₅	0.9804	0.0000	0.0000	0.0001	38.3839	0.0000	0.0000
H ₂ O	0.9804	99.9982	0.0193	0.0039	0.0000	0.0007	0.0000
Compressibility factor (Z)		0.0673	0.1218	0.1440	1.1971	0.1679	0.4959
Molar volume (m ³ /kmd)		0.0226	0.0408	0.0483	0.4013	0.0563	0.1662
Molecular weight		18.015	31.361	27.016	221.556	21.259	17.167
Density (kg/m ³)		798.610	767.886	559.526	552.155	377.657	103.273
Volume %		0.321	18.557	35.725	14.986	2.846	27.566
Phase mole %		0.972	31.075	50.601	2.554	3.457	11.341

TABLE 5.1

Adaptive Implicit Stability-Based Timestep Cutting-Test Results

Cutting Factor	Number of cuts	Number of timesteps	Number of iterations	Normalized total CPU time	Normalized CPU per iteration	Average fraction of implicit blocks
SPE 5:						
1.	0	270	893	1.00	1.00	0.0412
0.98	16	275	904	0.992	0.980	0.0365
0.95	8	275	910	0.997	0.979	0.0368
0.92	5	273	899	0.976	0.969	0.0326
0.90	6	277	895	0.962	0.961	0.0304
0.80	3	277	912	0.994	0.973	0.0338
0.70	2	278	911	0.981	0.961	0.0311
0.60	0	270	893	0.992	0.992	0.0412
SPE 3:						
1.	0	40	130	1.00	1.00	0.0781
0.95	10	40	131	0.985	0.976	0.0753
0.90	9	42	134	0.999	0.969	0.0694
0.80	7	43	137	1.015	0.961	0.0697
0.70	3	42	136	0.999	0.955	0.0735
0.60	1	40	130	0.988	0.988	0.0752
0.50	0	40	130	1.000	1.000	0.0781

TABLE 5.2
Fixed Map Stability-Based Timestep Cutting - Test Results for Explicit Map

Timestep selection method	Number of cuts	Number of timesteps	Number of iterations	Normalized total CPU time	Normalized CPU per iteration
SPE: 5					
Fixed Maximum (30 days) Stability	0	311	704	1.00	1.00
	356	445	922	1.42	1.09
SPE 3:					
Fixed Maximum (60 days) Stability	0	96	117	1.00	1.00
	159	164	179	1.60	1.04

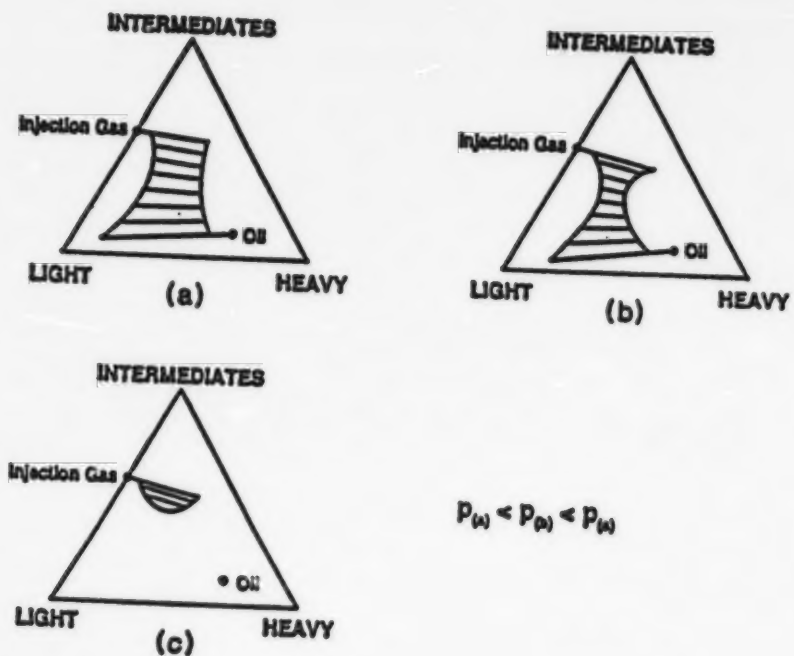
TABLE 6.1
Run-Time Comparison of Field-Scale Simulation

CO₂ Injection Process

<u>Run</u>	<u>Run-time ratio</u>
14 components, EOS flash calculations	5.76
4 components, EOS flash calculations	1.04
4 components, K-value correlation	1.00

Black-Oil Type Runs

<u>Run</u>	<u>Run-time ratio</u>
2 components, EOS flash calculations	2.30
2 components, K-value correlation	2.16
Black-oil simulator	1.00



$$P_w < P_o < P_w$$

Figure 2.1 - Pseudoternary diagrams for condensing/vaporizing gas drive

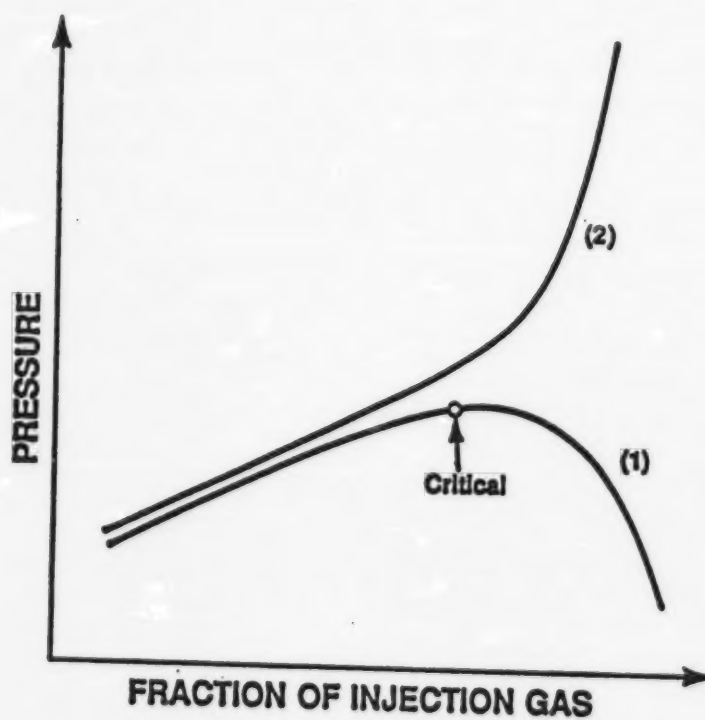


Figure 2.2 - Pressure-composition diagrams for gas injection processes

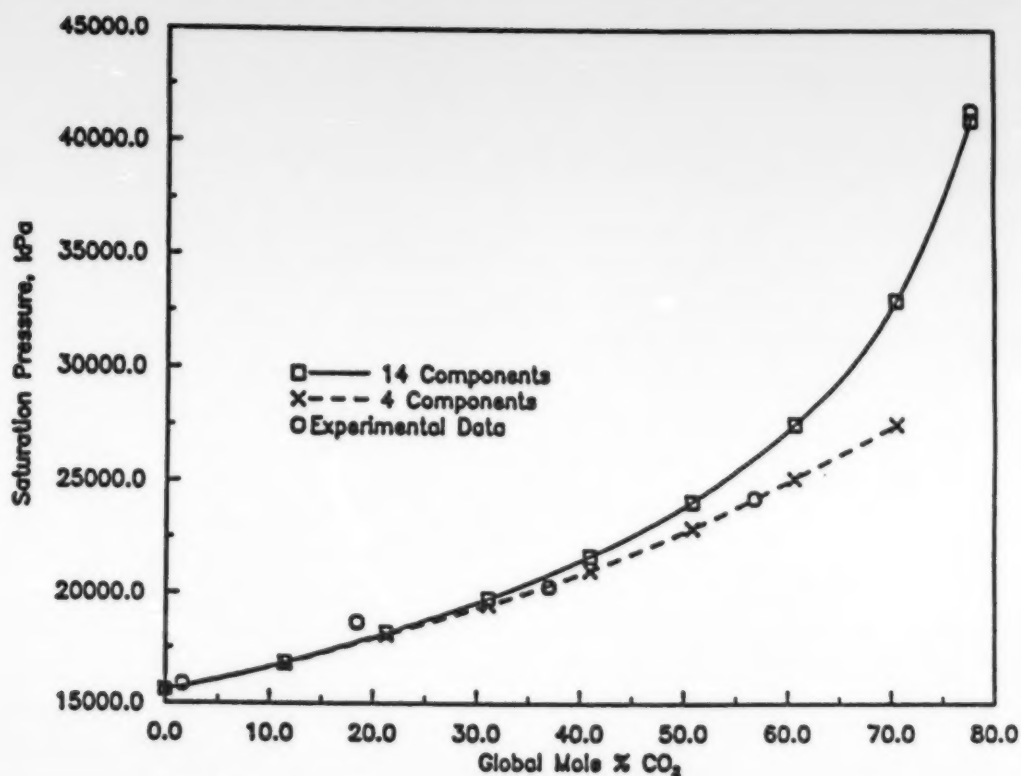


Figure 2.3 - Pressure-composition diagram for Sigmund et al (1979) oil with CO₂ injection

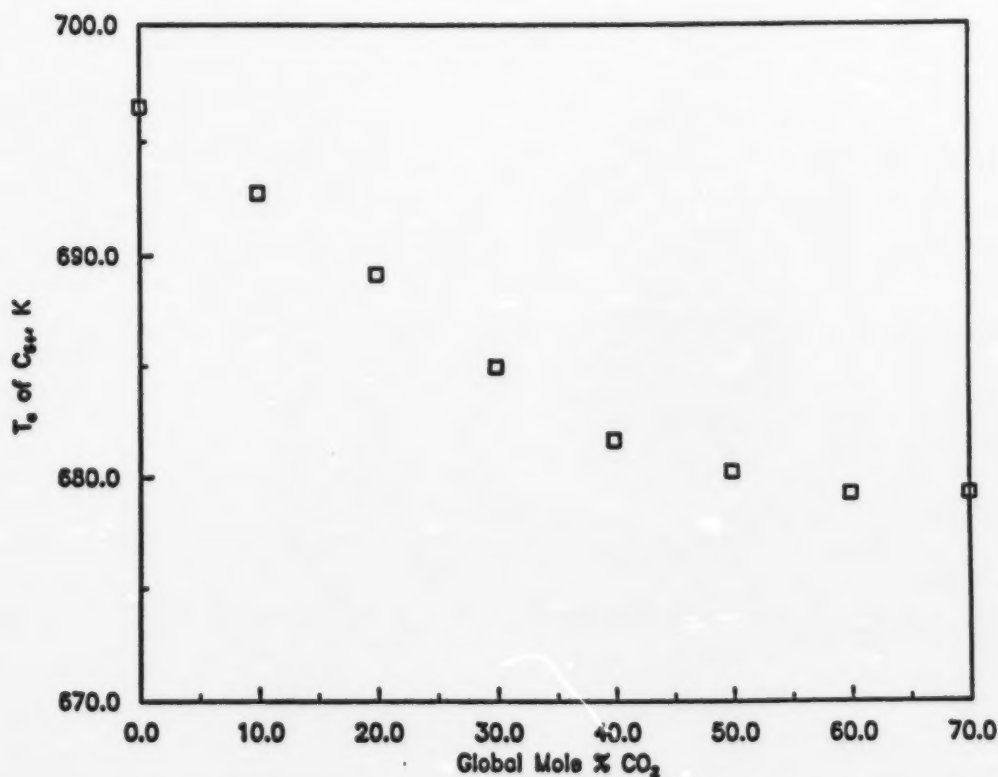


Figure 2.4 - Regressed critical temperature of C₄₊ fraction for few-component Sigmund et al (1979) oil with CO₂

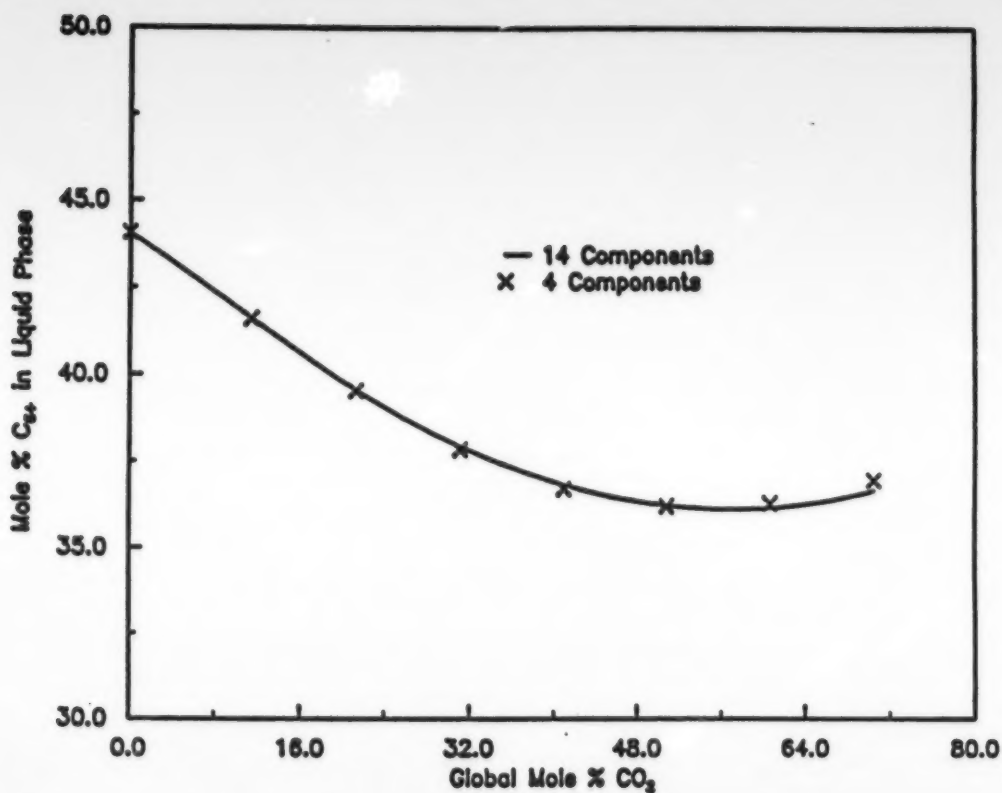


Figure 2.5 - Calculated composition of C_{6+} in liquid phase for many- and few-component Sigmund et al (1979) oil with CO_2

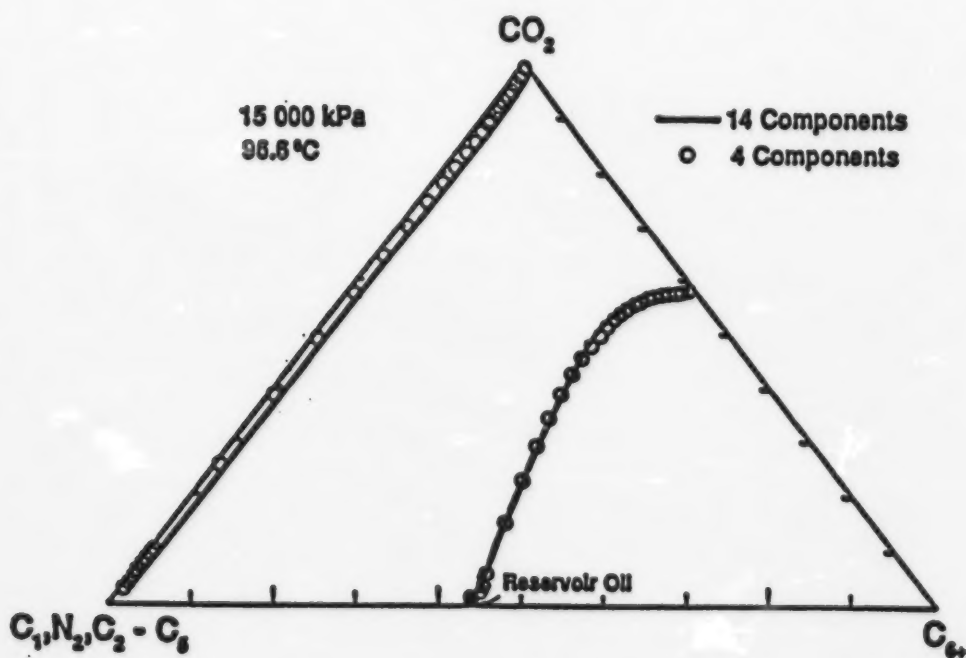


Figure 2.6 - Calculated pseudoternary diagrams for Sigmund et al (1979) oil with CO_2 injection at 15,000 kPa

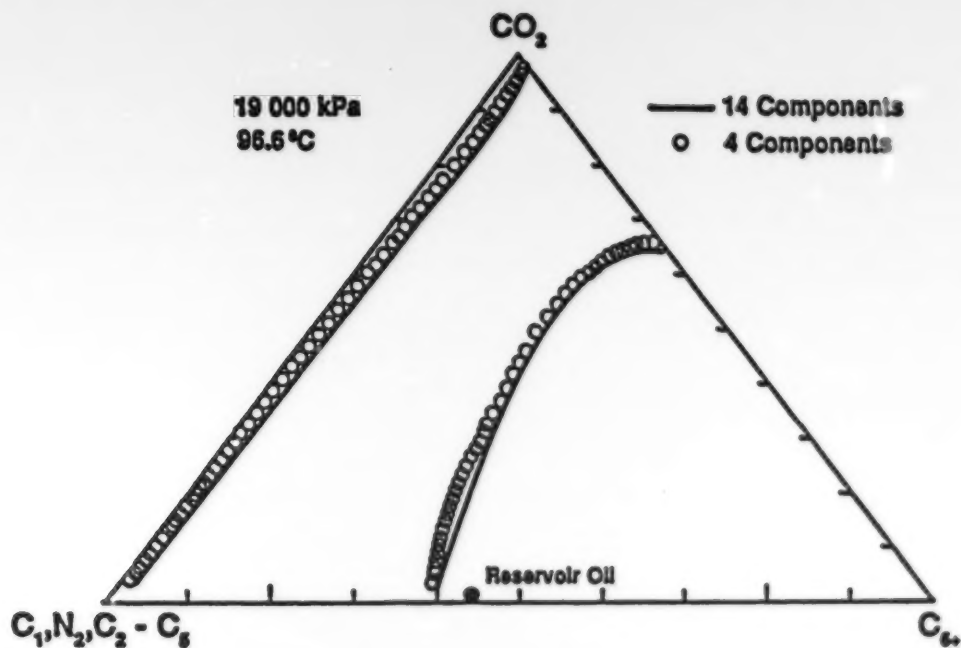


Figure 2.7' - Calculated pseudoternary diagrams for Sigmund et al (1979) oil with CO₂ injection at 19,000 kPa

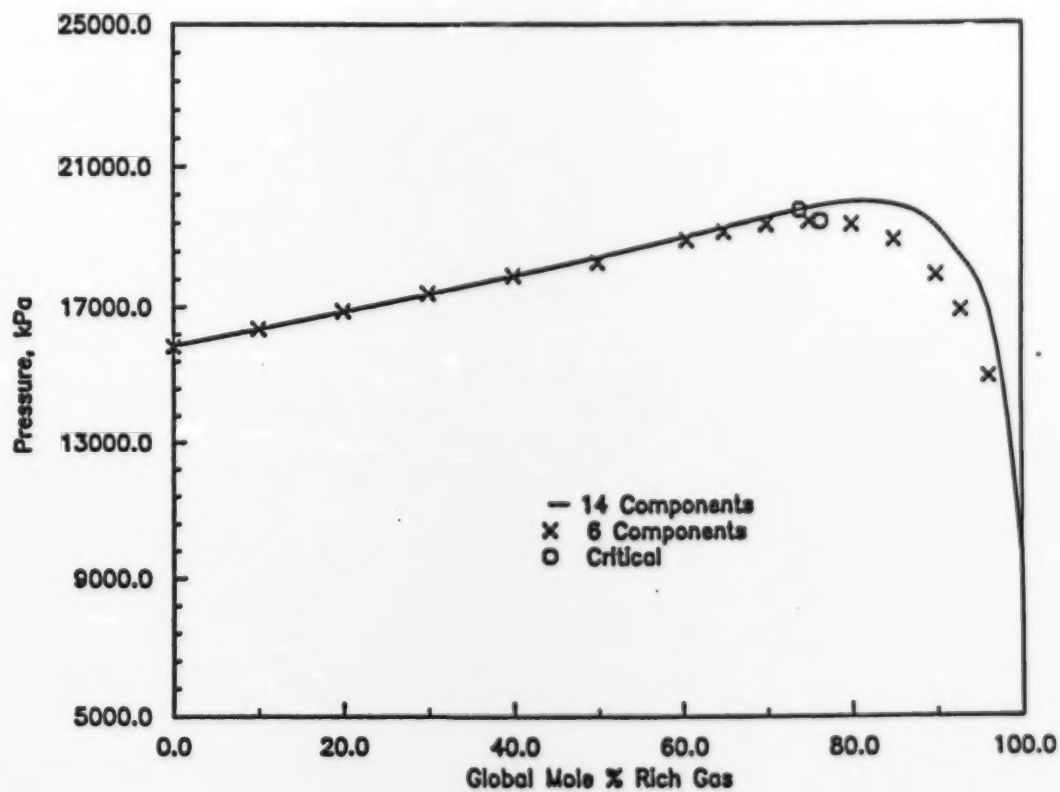


Figure 2.8 - Calculated pressure-composition diagram for Sigmund et al (1979) oil with rich-gas injection

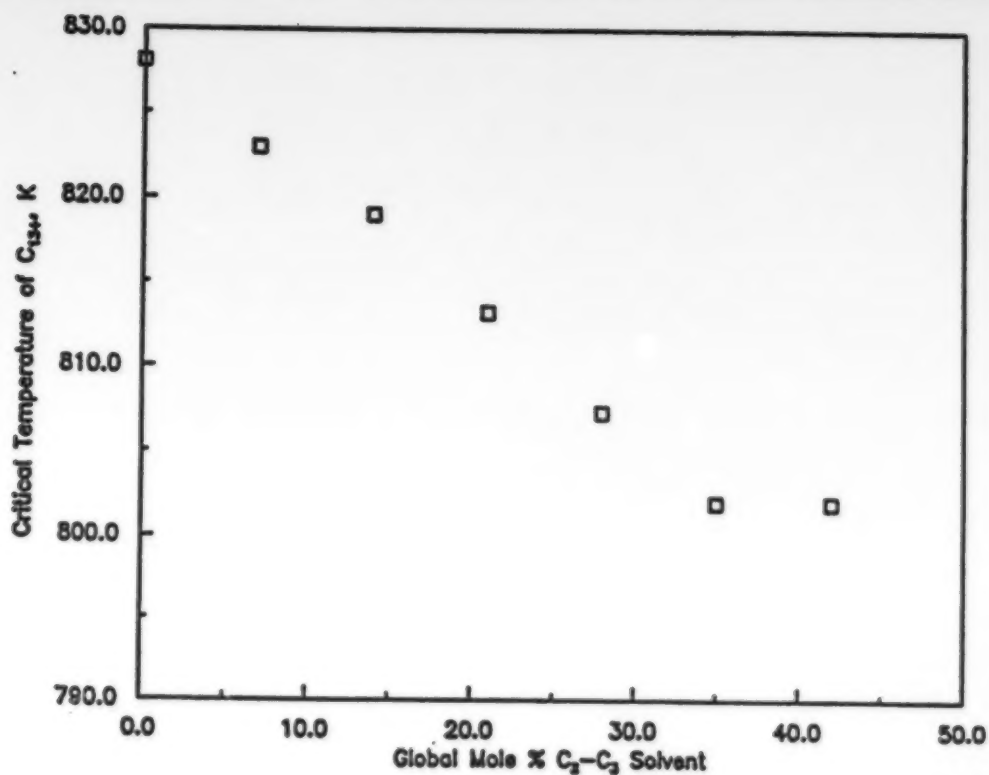


Figure 2.9 - Regressed critical temperature of C₁₃₊ for few-component Sigmund et al (1979) oil with rich-gas injection

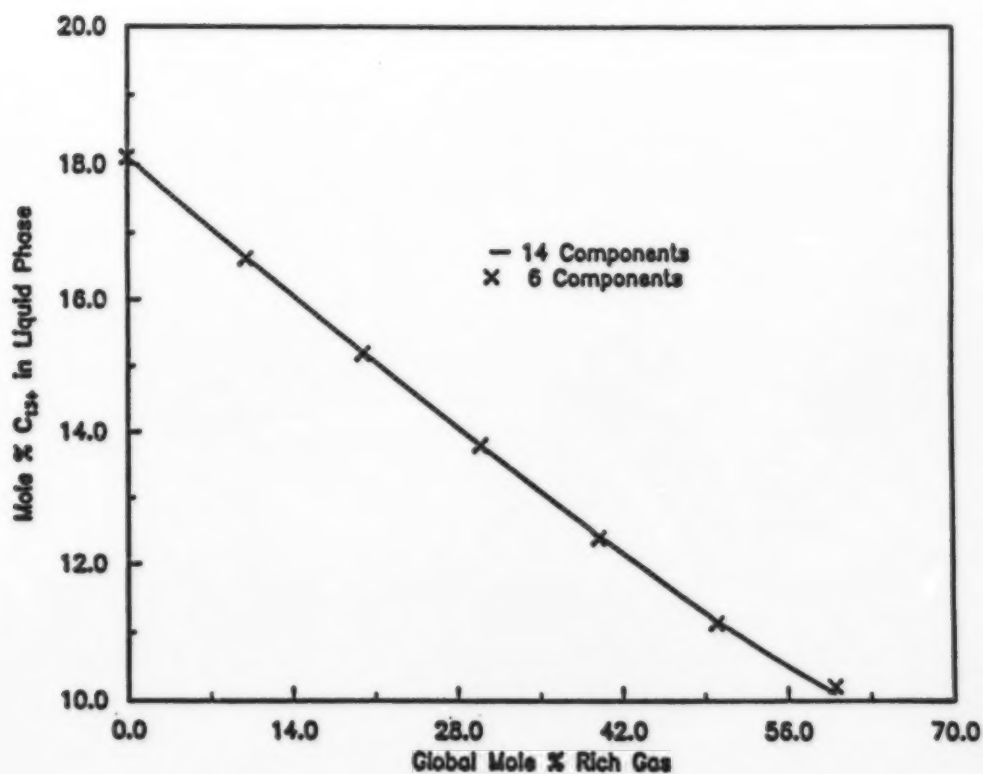


Figure 2.10 - Calculated C₁₃₊ composition in liquid phase for Sigmund et al (1979) oil with rich-gas injection

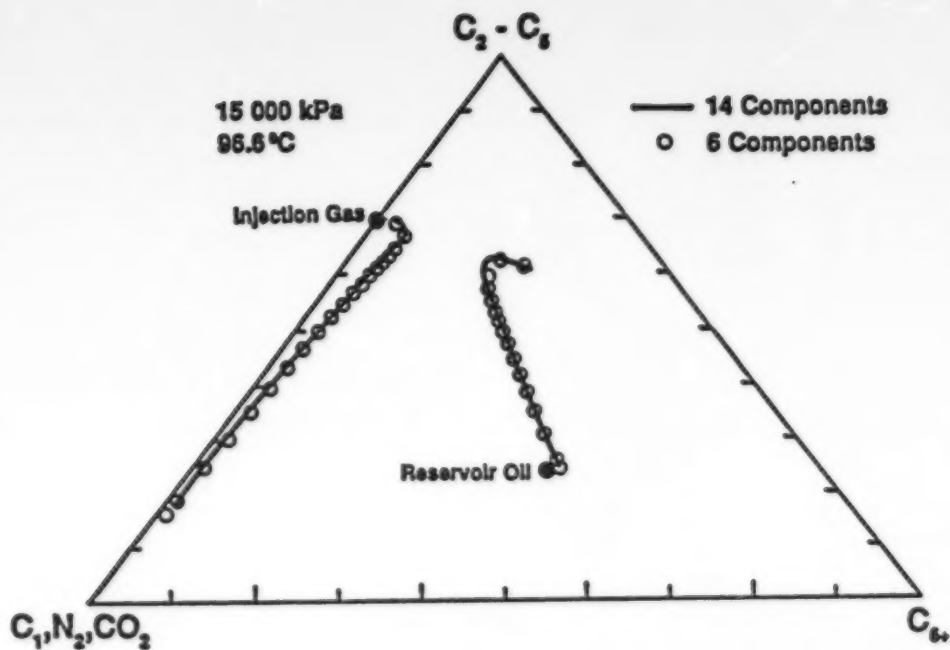


Figure 2.11 - Calculated pseudoternary diagrams for Sigmund et al (1979) oil with rich-gas injection at 15,000 kPa

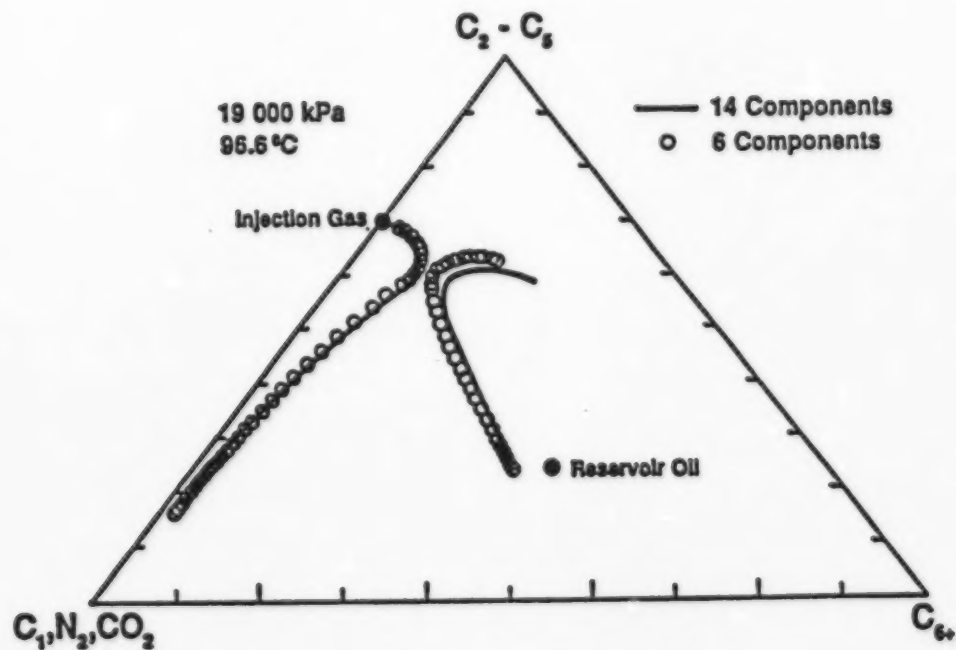


Figure 2.12 - Calculated pseudoternary diagrams for Sigmund et al (1979) oil with rich-gas injection at 19,000 kPa

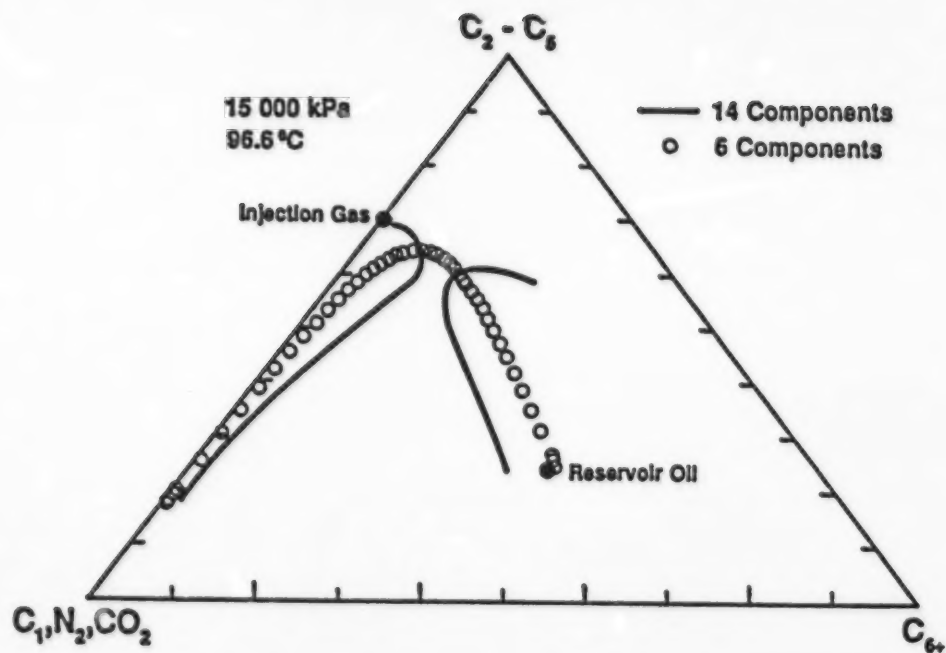


Figure 2.13 - Calculated pseudoternary diagram for 6 component Sigmund et al (1979) oil-rich gas system with only one C_{6+} component

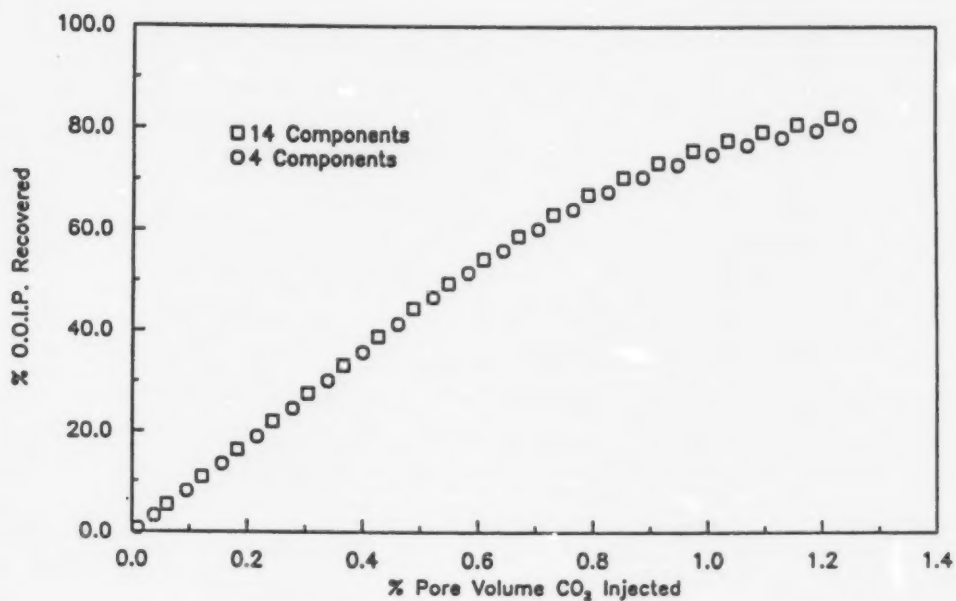


Figure 2.14 Slim-tube CO₂ displacement at 15000 kPa

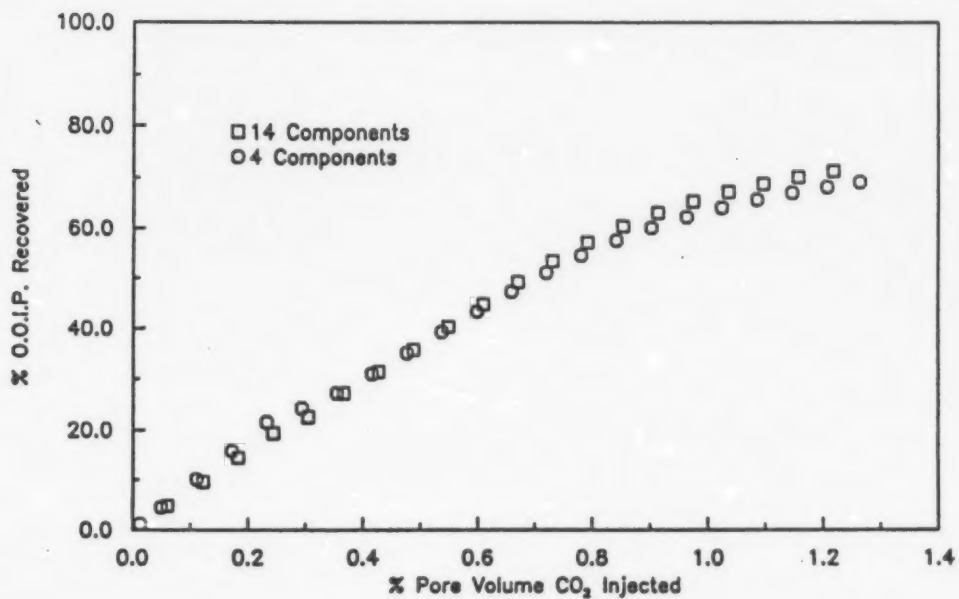


Figure 2.15 Slim-tube CO₂ displacement at 19000 kPa

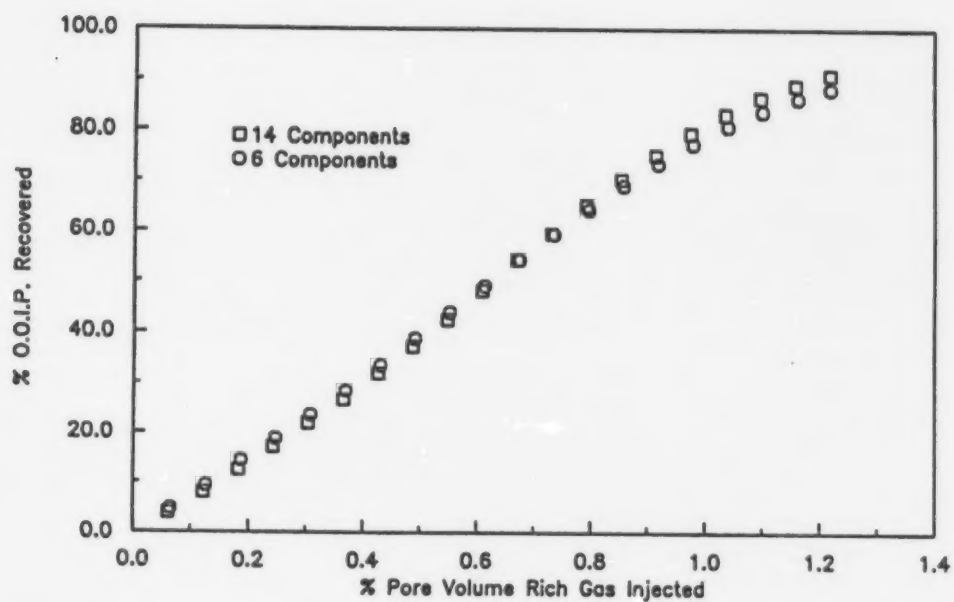


Figure 2.16 Slim-tube rich-gas displacement at 15000 kPa

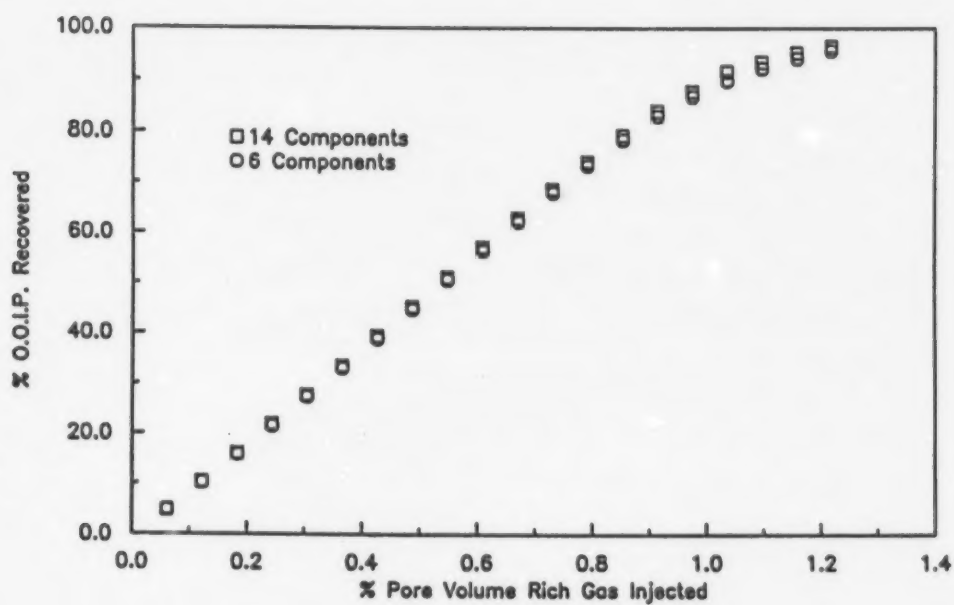


Figure 2.17 Slim-tube rich-gas displacement at 19000 kPa

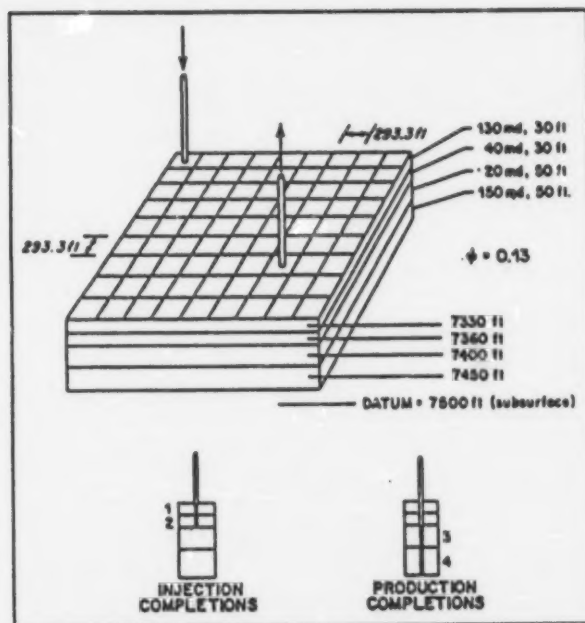


Figure 3.1 Third comparative solution project 9x9x4 reservoir model grid

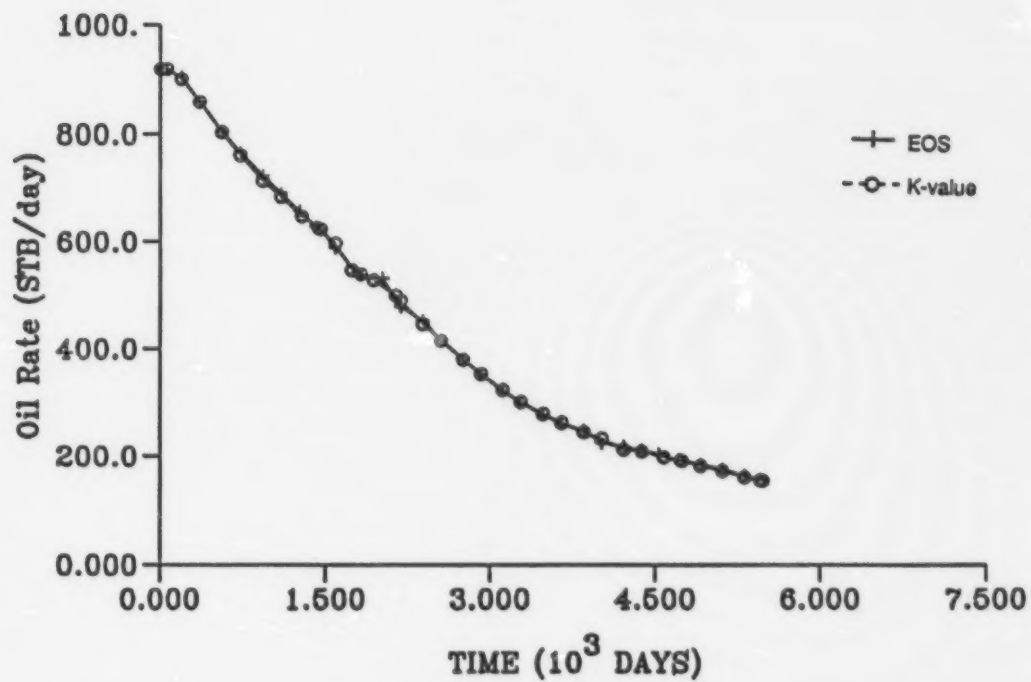


Figure 3.2 Comparison of oil rates

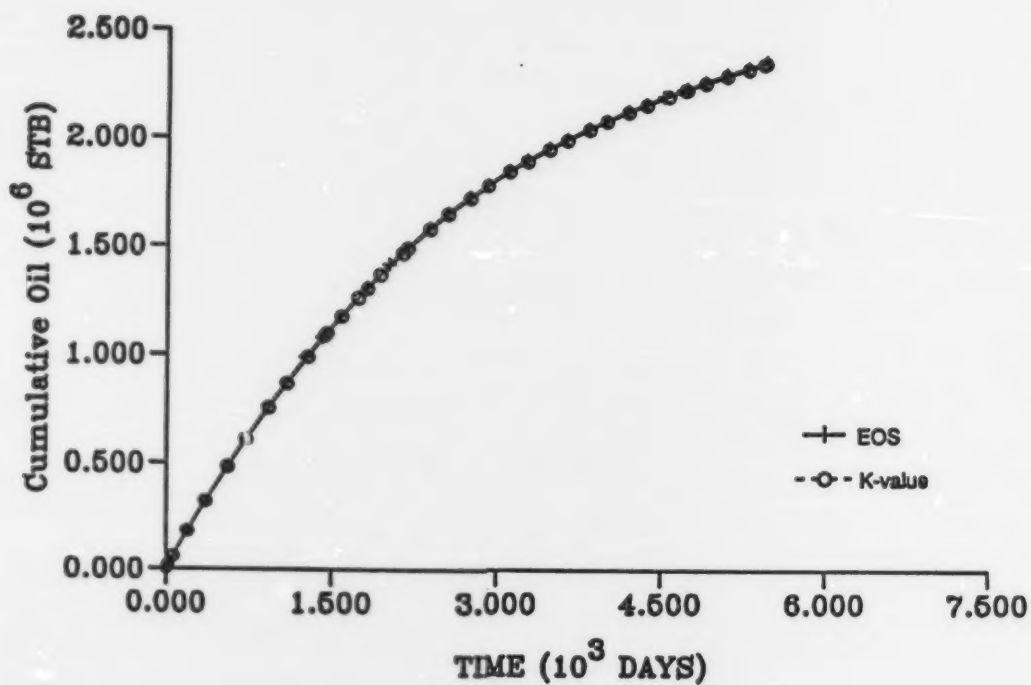


Figure 3.3 Comparison of cumulative oil production

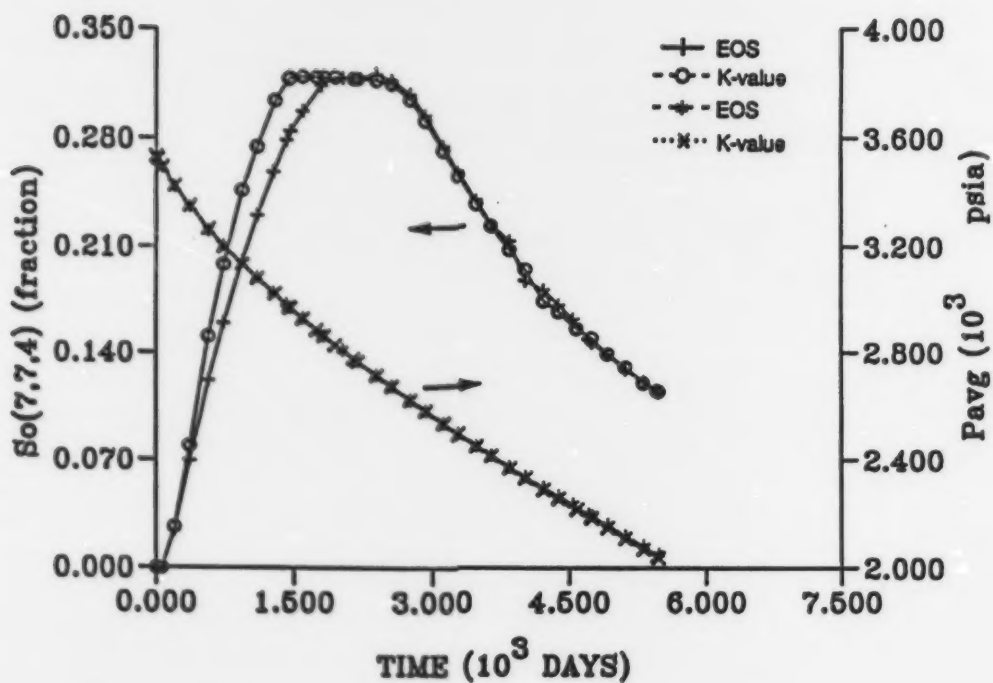


Figure 3.4 Comparison of oil saturation in Gridblock (7,7,4) and average reservoir pressure

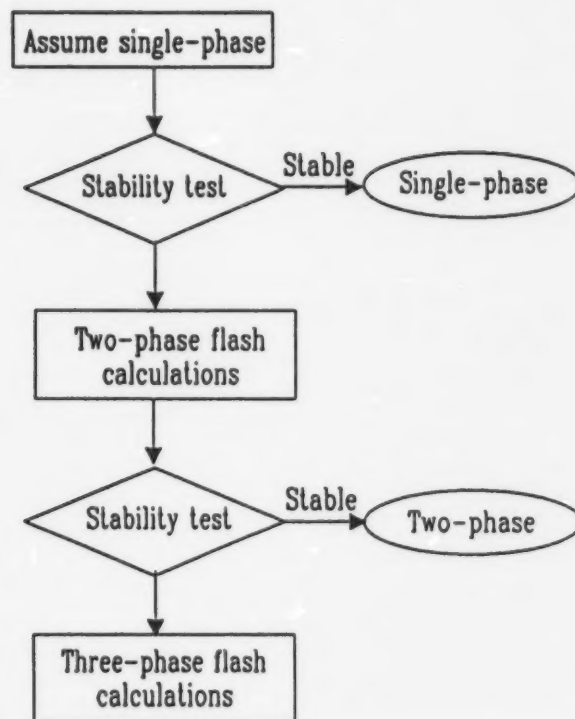


Figure 4.1 Stagewise procedure for three-phase flash calculations with stability tests

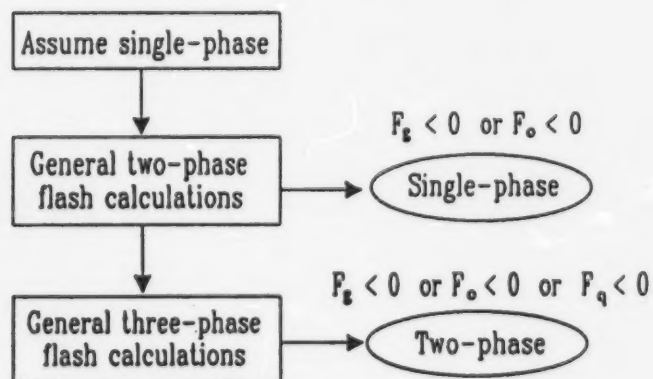


Figure 4.2 Stagewise procedure for general three-phase flash calculations

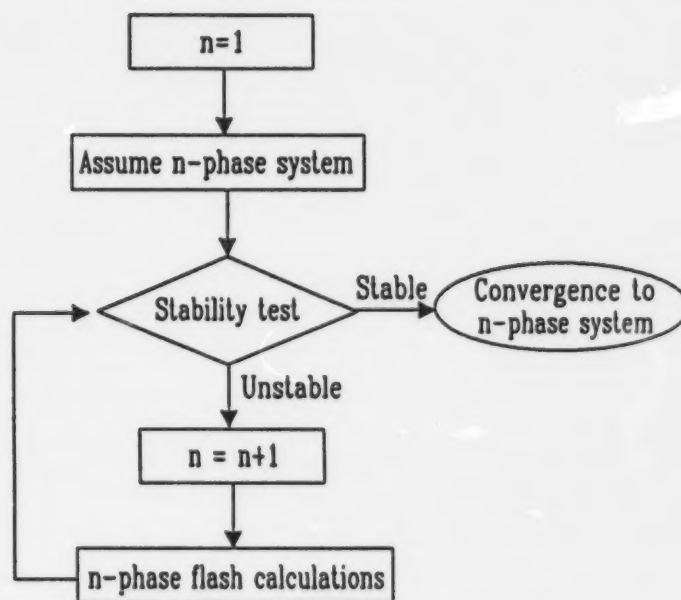


Figure 4.3 Stagewise procedure for n-phase flash calculations with stability tests

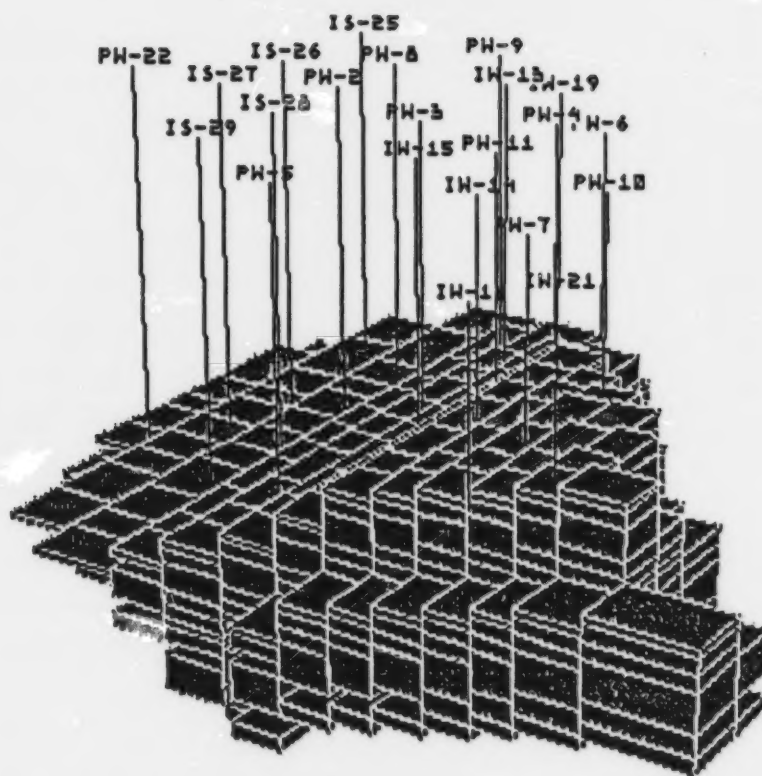


Figure 6.1 Reservoir for field scale runs

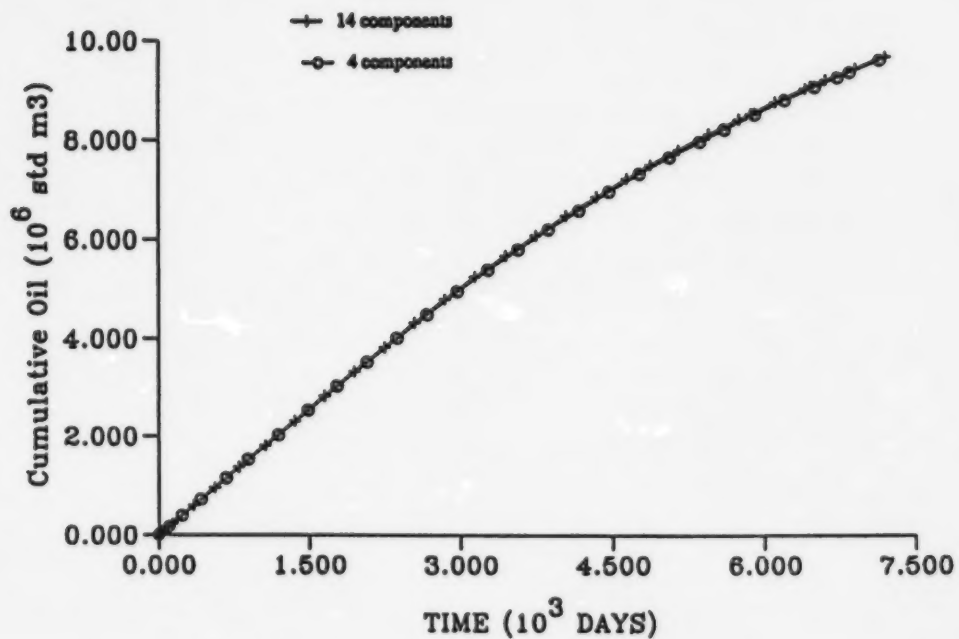


Figure 6.3 Field-scale CO₂ Injection - Cumulative oil production

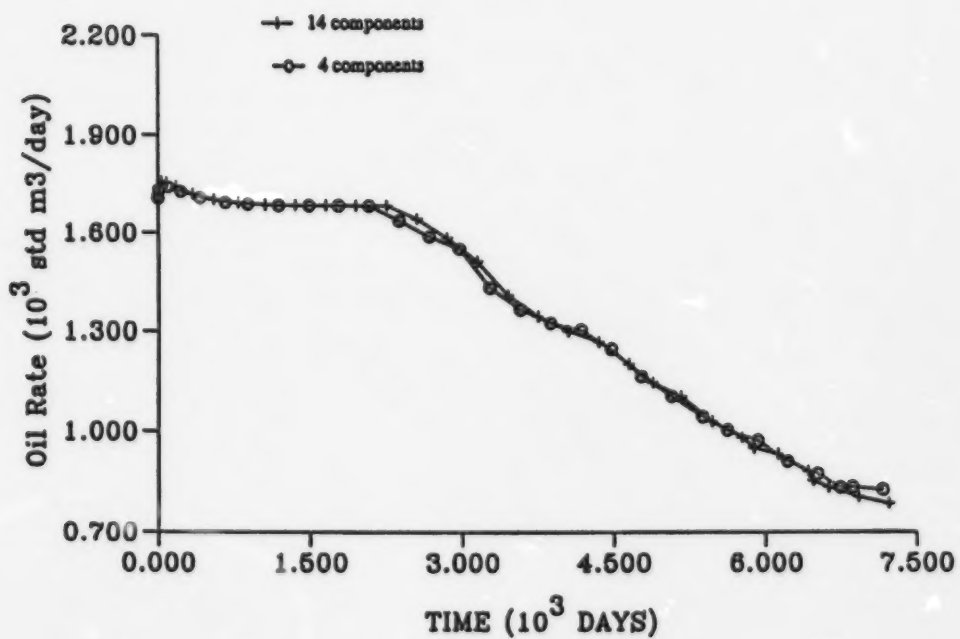


Figure 6.3 Field-scale CO₂ Injection - Total oil production rate

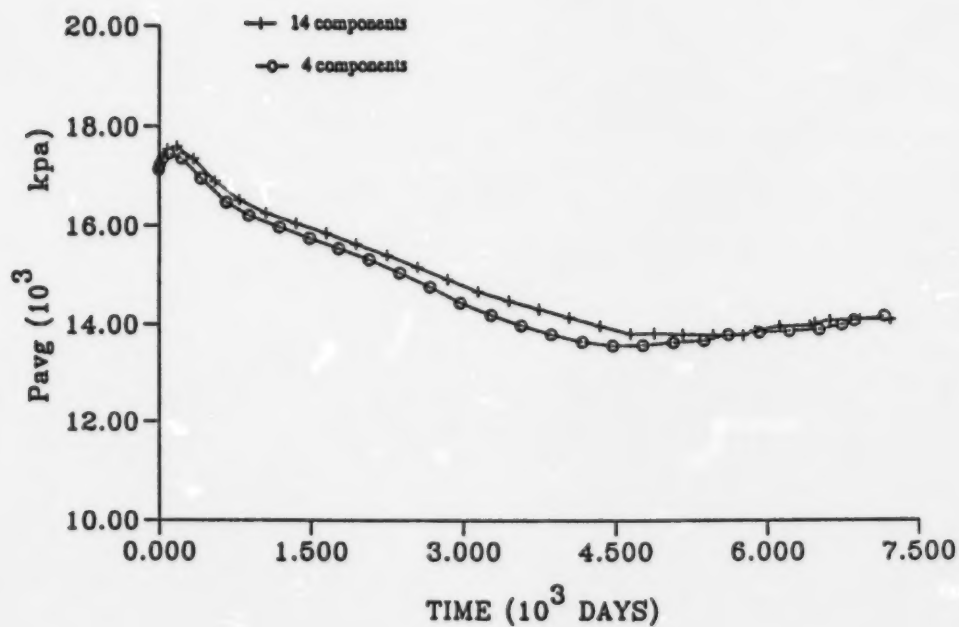


Figure 6.4 Field-scale CO_2 Injection - Average reservoir pressure

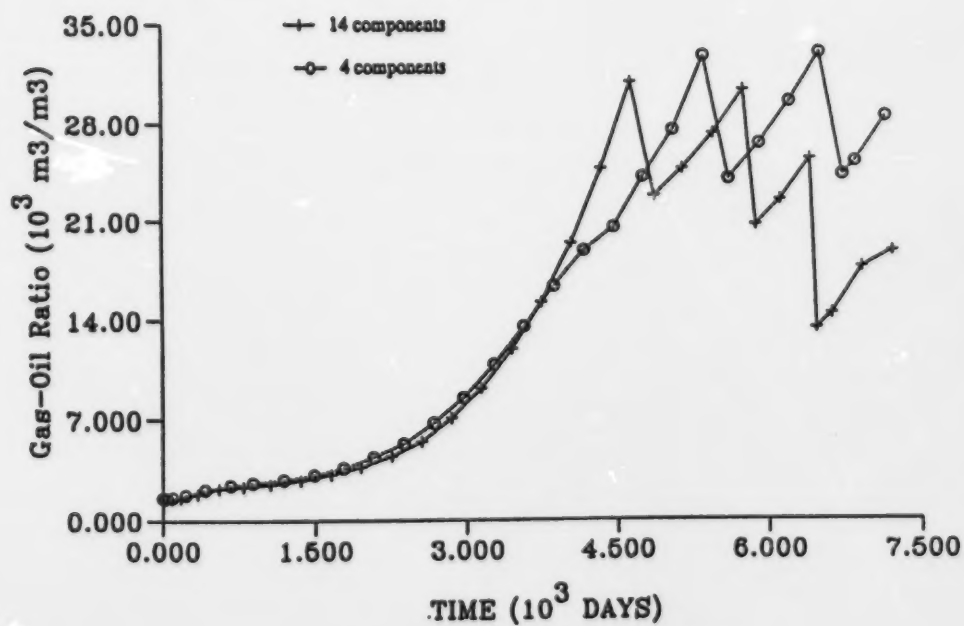


Figure 6.5 Field-scale CO_2 Injection - Gas oil ratio

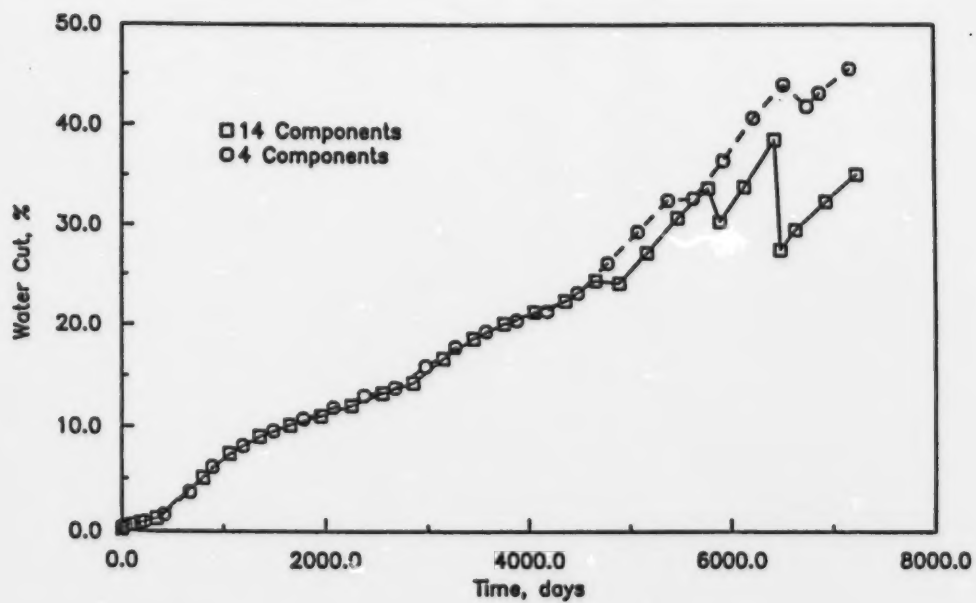


Figure 6.6 Field-scale CO₂ Injection - Water cut

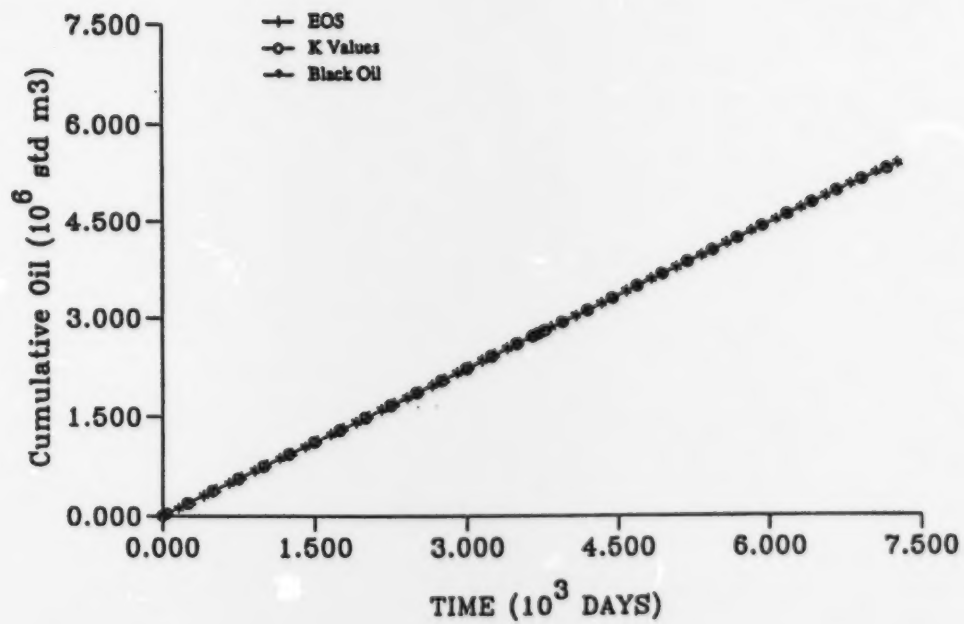


Figure 6.7 Field-scale black-oil run - Cumulative oil production

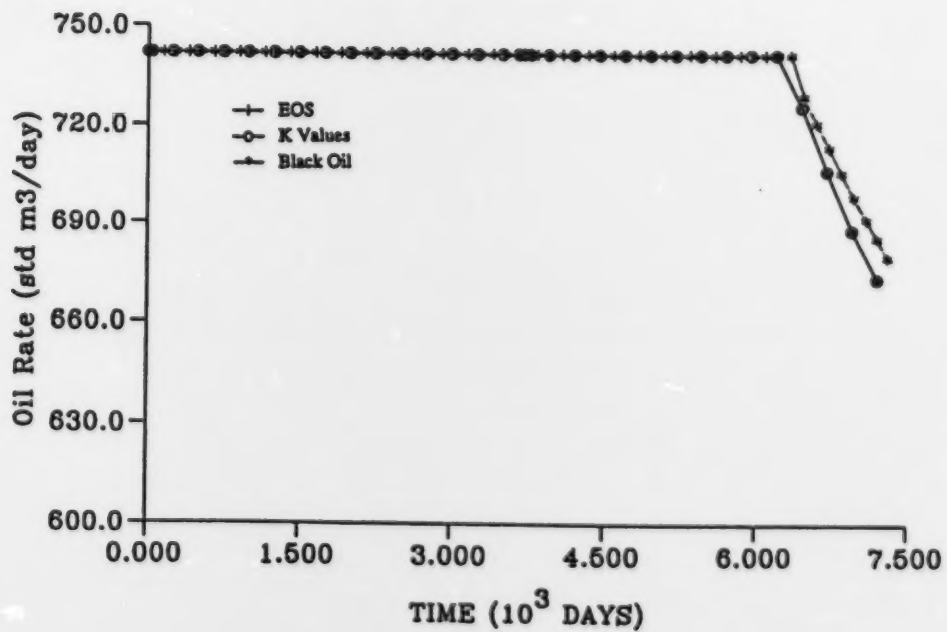


Figure 6.8 Field-scale black-oil run - Total oil production rate

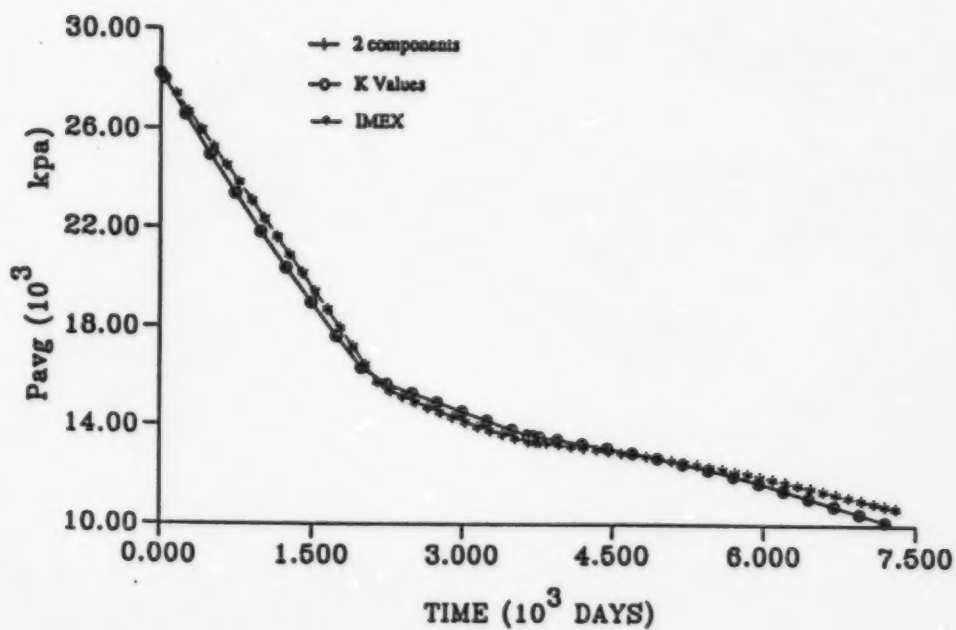


Figure 6.9 Field-scale black-oil run - Average reservoir pressure

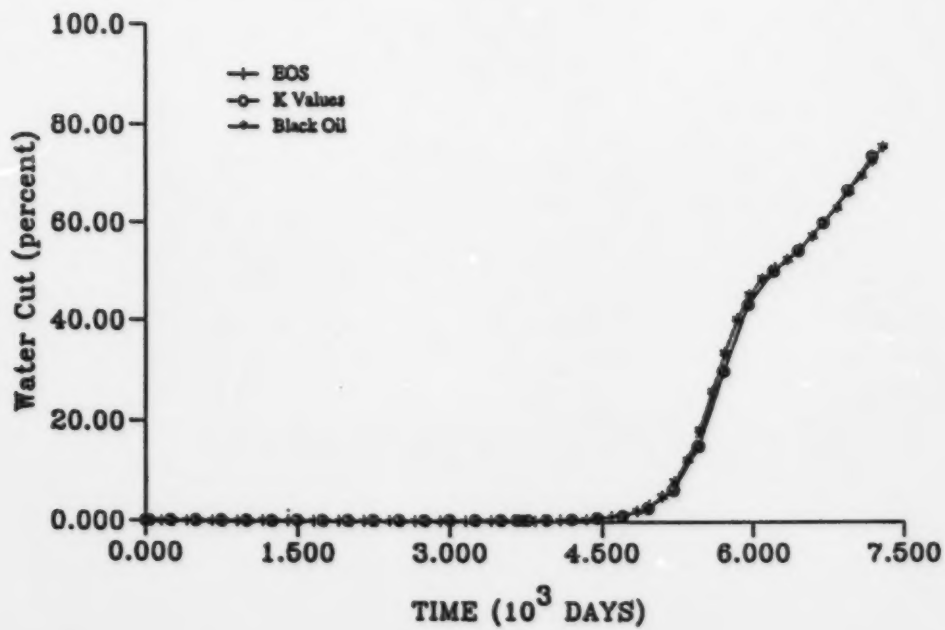


Figure 6.10 Field-scale black-oil run - water cut